Mediterranean chemometrics

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Published online: 23 December 2010

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Since the proposal of the term “chemometrics” by S. Wold, in 1972, there have been many attempts to provide a definition which clearly identifies its objectives, methods, and results. One of the most recent definitions states that *chemometrics is the science of relating measurements made on a chemical system or process to the state of the system via application of mathematical or statistical methods* (Anal Chim Acta (2009) 642:3–5). However, in our opinion, this definition has a major shortcoming—it does not mention the measurement process, which is intimately associated with the future use of the results of the measurement.

We tend to agree with the proposal of J. Workman that identifies chemometrics as a process which can solve routine chemical problems in different stages (J. Workman Jr. Chemometr Intell Lab Syst (2002) 60:13–23):

1. *measure a phenomenon or process by using chemical instrumentation that generates data inexpensively;*
2. *analyze the multivariate data;*
3. *iterate if necessary;*
4. *create and test the model; and*
5. *develop fundamental multivariate understanding of the process*

Published in the special issue on *Chemometrics (VII Colloquium Chemicum Mediterraneum)* with Guest Editors Juan M. Bosque-Sendra and Luis Cuadros-Rodríguez

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Current chemometrics implies chemistry, mathematics (statistics), and process measurement (sensors).

This chemometric approach to chemical knowledge is a consequence of the multivariate nature of major chemical systems, so univariate methods are unable to provide optimum solutions, as was established in the anthological report by K.S. Booksh and B.R. Kowalski in which the fundamentals of the Theory of the Analytical Chemistry were stated (Anal Chem (1994) 66:782A–791A). Current analytical instrumentation and chemometrics let us see the world from a multivariate perspective and, in this sense, mathematics are not used to model, per se, processes or phenomena but to establish hidden relationships between the data and the state of the system under study, as is stated in the definition cited above. The division between univariate and multivariate data opens the way for the development of chemometrics, so this science can be summarized in one word: multivariate, and it is precisely the development of chemometrics, mainly in multivariate optimization, pattern recognition (classification and modeling), and calibration, which supports the basis of current analytical chemistry.

From its beginning, chemometrics has been extended in many directions, for example in well-established applications. We could quote examples as food authentication, process analytical technology (PAT), environmental monitoring, geological data analysis, or cultural heritage knowledge. Extensive information about chemometrics can be found in the recently published four-volume encyclopedia entitled “Comprehensive Chemometrics” which is intended to be a reference textbook among scientists and researchers in the field. Modern chemometrics has sought new applications in a wide range of fields, some very far from chemistry. We highlight three of these, chemoinformatics, image analysis, and “omics” sciences, as the most relevant examples.

In chemoinformatics, which can be regarded as a branch of chemometrics, analysis, visualization, and structural chemical information are used with purposes such as quantitative structure–property relationships (QSPR), quantitative structure–activity relationships (QSAR), or drug design. Image analysis is a combination of molecular spectroscopy (using any type of electromagnetic radiation) and digital image processing. The use of cameras and image sensors can produce large data sets that require the use of specific tools similar to those used in classical chemometrics.

Recently, many fields of study related to system biology have been developed. They have in common the “omics” ending in their name (proteomics, genomics, metabolomics, lipidomics, foodomics, ...). The main objective of these fields is the study of the effects of different types of treatments and conditions on biological systems. These studies have led to the need for tools to deal with large amounts of very complex data supplied by the instrumental system. Chemometrics has found huge scope. Although, P. Geladi, has warned about a problem, which is more apparent than real, the “omics” sciences can absorb chemometrics, or at least chemometricians (J Chemom (2008) 22:289–290).

In Europe, chemometrics started in the Scandinavian countries (in northern Europe) where S. Wold was born. From its beginnings, there were two additional chemometric cores in Europe, one located in the center of the continent, whose representative countries are the Netherlands and Belgium, and another in southern Europe which initially focused on Italy but has spread mainly to Spain. The existence of competitive research groups in these countries has helped to preserve a high level of development. This has been reinforced by the holding of conferences on chemometrics. For example, the Scandinavian Symposium on Chemometrics (SSC), launched in 1989, and which celebrates its twelfth meeting in 2011, or the Annual Symposium on Chemometrics and the International Chemometrics Research Meeting (ICRM), both organized by the Dutch Chemometrics Society, which had their 27th and 4th meetings, respectively, in 2010.

In the Mediterranean basin, Italy, Spain, and France have been organizing a cyclical series of conferences with the Latin denomination Colloquium Chemiometricum Mediterraneum (CCM). This meeting has as its origin celebration of the conference “Chemometrics in Analytical Chemistry (CAC III)” in Lerici (Italy, 1986), when a group of chemometricians from France, Spain, and Italy gathered to share their experience and knowledge in their own languages. This was the germ of CCM. Since then, this meeting has maintained continuity under the impulse of Professor M. Forina of the University of Genoa (Italy), beginning with the first meeting in Barcelona (Spain, 1987), and then successively in San Miniato (Italy, 1991),

Bastia (France, 1994), Burgos (Spain, 1998), Ustica (Italy, 2003), and Saint Maximin La Sainte-Baume (France, 2007). The participation rules are simple and have been preserved in all meetings. The participants present their work in their own language (an officially recognized Romance language, mainly French, Italian, or Spanish) but with audiovisual support in English.

The “VII Colloquium Chemiometricum Mediterraneum (CCM VII)” with the motto: *propinat opportunitatem exiniam ad intermutandum cognitiones a novitatibus collocatis in cuspide et rerum novarum* (it offers an outstanding and unique opportunity for exchanging knowledge on leading edge developments) was held from 21th to 24th June 2010 in Granada (Spain). The Colloquium comprised nine sessions of oral presentations and two sessions of poster communications and included six plenary lectures given by researchers from Spain, Italy, and France, plus another two given by non-Mediterranean lecturers with international prestige on the subject. The invited lecturers were: Michele Forina (University of Genoa, Italy), Rasmus Bro (University of Copenhagen, Denmark), Age Smilde (University of Amsterdam, The Netherlands), Max Feinberg (National Institute of Agronomic Research, Paris, France), Roberto Todeschini (University of Milan, Italy), Luis Sarabia (University of Burgos, Spain), Michelle Sergent (University of Marseille, France), and Anna de Juan (University of Barcelona, Spain). The conference was attended by 150 researchers from 12 European, mainly Mediterranean, and Latin American countries, and a total of 29 oral communications and 112 posters were presented.

On the last day of the congress an emotional tribute was paid to Professor M. Forina, on the occasion of his forthcoming retirement. The ceremony was attended by many colleagues and collaborators. Among these can be mentioned the contributions of Professors R. Phan-Tan-Luu (University of Marseille, France—now retired), L. Sarabia (University of Burgos, Spain), and C. Pizarro (Universidad de La Rioja, Spain). Professor M. Forina has always been characterized by his support of Mediterranean science within Europe, and by his constant academic and research activities since 1988 in the field of chemometrics. This special issue which collects, as research papers, some of the main contributions presented at the VII Colloquium Chemiometricum Mediterraneum (CCM VII) is dedicated to him.

We are especially very grateful to *Analytical Chemistry and Bioanalytical* for the opportunity to publish these papers. This journal, in its relatively short life, has always shown a great interest in chemometrics, as is evident from the special issues that readers can find in volumes 372/ (2002), 380/3 (2004), 390/5 (2008), and this volume. These issues and the numerous articles published in them give a complete overview of the development and progress of chemometrics in the first decade of the twenty-first century.

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