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Chemometrics in Argentina: the Result of Unplanned Events

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Apresenta-se breve relato sobre a história da quimiometria na Argentina, desde a criação da Associação Argentina de Químicos Analíticos em 1999, que possibilitou um esforço conjunto para o desenvolvimento mais sistemático da disciplina no país, até os dias atuais, com vários grupos pesquisando sobre diferentes temas em quimiometria.

A brief account is provided on the history of chemometrics in Argentina, from the creation of the Argentinean Association of Analytical Chemists in 1999, which created the opportunity of joining efforts for a more rational development of the discipline in the country, to the present days, with a variety of groups conducting research in several different aspects of chemometrics.

Keyword: chemometrics, historical evolution, Argentina

1. Introduction

In 1999 the Argentinean Association of Analytical Chemists (AAQA, http://www.aaqa.org.ar/) was founded in the city of San Luis, by a group of analytical chemists from all over the country. The National University of San Luis held the most active research group on analytical chemistry, and it is thus understandable that the first impulse for the creation of the association came from them. It was a long-sought aim of various members of several research groups, which were rather dispersed across the country and with little communication among them. The purpose of the AAQA was to organize scientific meetings in such a way that the communication gap was closed as much as possible, to promote the development of Analytical Chemistry throughout the country, and to encourage young people to join the Association and pursue the discipline.

That initial effort proved to be highly successful. Today the AAQA has hundreds of members, has promoted and financed post-graduate courses in different universities, and has already organized six national scientific meetings; the seventh one was held at the city of Mendoza in October 2013 (http://www.uncu.edu.ar/7cqa/). One of these meetings, held in Buenos Aires in 2007, was at the same time the III Ibero-American Congress on Analytical Chemistry. The AAQA meetings are now regularly organized every two years in different Argentinean cities, with a continuously increasing number of participants and work presentations, and with the contribution of distinguished foreign researchers as lecturers, organization of round tables on various subjects (education, connection with industry, etc.), and active and enjoyable social programs. A particularly important aspect is that every AAQA meeting brings several foreign invited speakers, whose subject are distributed among the main areas of analytical chemistry research, i.e., spectroscopy (molecular and atomic), electrochemistry, chromatography, and most importantly, chemometrics. In previous meetings, lectures in chemometrics have been given by Romà Tauler (Barcelona, Spain), Bernhardt Lendl (Viena, Austria), Arsenio Muñoz de la Peña (Badajoz, Spain), and Marcel Maeder (Newcastle, Australia).

One particular event triggered by the foundation of the AAQA concerns chemometrics. At the founding meeting in San Luis in 1999, researchers working in different aspects of chemometrics, who did not know each other personally, found themselves in the same place, talking about common issues. After this event, a series of other, more causally connected facts occurred. The chemometricians decided to join efforts in promoting the discipline, by giving courses (both personal and electronic) in different universities, to receive young researchers with chemometric interests in their laboratories, and to invite well-known

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chemometricians from abroad to give courses, or lectures at the AAQA congresses, among other actions.

As a result of the particularly fortuitous occasion in 1999, therefore, the current situation of chemometrics in Argentina is significantly better than before. It is, however, far from being ideal, but considerable progress has been made. The three main chemometric areas of interest are now being pursued in several laboratories: (*i*) design of experiments and optimization, (*ii*) multivariate calibration and (*iii*) sample discrimination and classification. In what follows some representative works in these areas will be mentioned, including the cities in which the researchers work.

2. Design of experiments and optimization

The need of rationally designing experiments in order to assess the relevant factors affecting a given response, and the importance of optimizing an objective response using statistical techniques is now fully appreciated by most members of the chemistry community in Argentina. Some groups (Santa Fe and Buenos Aires) devote efforts to develop new screening tools, based on genetic algorithms applied to Plackett-Burman designs,[1,2] or optimization methodologies based on the use of artificial neural networks.[3,4] Other groups have included design and optimization as an integral part of analytical method development, particularly when multiple factors are involved, as in capillary electrophoresis or liquid-liquid extraction procedures (Santa Fe, Buenos Aires, Mendoza).[5-7] In other cases, optimization is the final aim, as in the design of new pharmaceutical delivery systems (Rosario).[8,9]

3. Classification and discrimination

Classification of samples using various techniques (principal component analysis, artificial neural networks, etc.) is a subject which is being pursued at several laboratories. The purposes are as diverse as the control of foodstuff such as honey,[10] garlic[11] and seeds (La Pampa, San Luis),[12] wine[13,14] and wheat (Córdoba),[15] the study of material properties (Buenos Aires),[16] the development of electronic noses (Buenos Aires),[17,18] etc. Related techniques based on artificial neural networks have been applied to study patients in neutron capture therapy[19] or sources of environmental pollution (Buenos Aires).[20]

4. Multivariate calibration

In the area of multivariate calibration, complex sample analysis using first-order spectroscopic methods coupled to partial least-squares regression (PLS) and other variants has been the interest of several groups. Only as examples, work has been done on therapeutic drugs both in pharmaceutical forms and biological fluids, metals, foodstuff and environmental samples (Santa Fe, La Pampa, San Luis, Bahía Blanca, Rosario, Buenos Aires).[21-27] In this area, not only applications have been made, but also theoretical developments, such as variable selection using a variety of new algorithms (Santa Fe, Bahía Blanca, Rosario),[28-30] sample selection (Santa Fe, Buenos Aires),[31,32] new calibration methodologies based on net analyte signals (Santa Fe, Rosario),[33] calibration transfer and maintenance (Santa Fe),[34] etc.

Second- and higher-order calibration, i.e., using matrix data or higher-order arrays, is the subject of interest of a few groups today, but will undoubtedly grow in the future, as the chemical instrumentation becomes more complex. The need of processing and interpreting the huge amount of data provided by these instruments will certainly trigger increasing developments and awareness of the possibilities offered by them. Applications have been made by a number of groups (Santa Fe, Bahía Blanca, La Plata, Rosario), and referred to analysis in environmental samples,[35-37] foodstuff,[38] biological fluids,[39] pharmaceuticals,[40,41] sediments,[42] etc. New developments in the estimation of figures of merit have been recently published (Rosario).[43]

5. QSAR

Another important area of chemometric studies is quantitative structure-activity and property relationship (QSAR/QSPR), with some groups developing methods for correlating various biological and other important properties with molecular descriptors (San Luis, La Plata).[44-48]

6. Conclusions

Somewhat ironically, the San Luis researchers who organized the founding meeting for the AAQA have analytical research interests in two areas which are in less need of chemometric assistance: atomic spectrometry and specific electro-analytical sensors. It is a nice example of serendipity, because the unplanned first brick laid by the San Luis group in 1999 gave rise to the growing construction of the chemometric discipline of today.

A long way is expecting us in the future. Some proposals for increasing the strength of chemometrics in Argentina follow, partly by consideration of the short story told above, partly by looking at what other countries have done in the past, especially Brazil. The first advice for scientific

policy makers of our country is to avoid randomness to be the cause of the development of any discipline, including chemometrics. We need planning, and by planning I mean several political actions that should be taken by authorities: advanced courses on chemometrics should not be the result of the personal effort of individuals but officially organized and supported, introduction of the discipline in the curricula of the Chemistry-related careers (Chemistry, Biochemistry, Biotechnology, Pharmacy, etc.) should not be left to the random existence of experts in a given university, but should be suggested by some national board to all universities, fellowships and grants should be available to chemometric-oriented research with a certain priority, etc.

Another proposal aimed at improving the development of chemometrics in Argentina is the promotion of international contacts. Cooperation projects with major universities and research centers of USA and Europe should be stimulated, young people should be supported if they intend to learn advanced chemometrics in the world's most prestigious laboratories. Experts from those centers should be invited to Argentina to give lectures, courses, seminars, etc. A particularly successful example in this regard is the Chemometrics Winter School held from August 26 to August 30, 2013, in the Federal University of São Carlos, Brazil, successfully organized by Profs Edenir Rodrigues Pereira Filho and Renato Lajarim Carneiro. The assistance of ca. 150 graduate and post-graduate students from all over Brazil is a proof of their success. Lectures and courses from Brazilian chemometricians and researchers from USA, Europe and Argentina during that particular week were possible in an atmosphere of both friendship and scientific progress.

Finally, regional cooperation among South American countries should be encouraged, with a two-fold purpose: to learn from the most advanced ones, and to help the less developed. Political decisions and real actions in this field are needed, as part of a higher aim: the integration of all American brothers.

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