

Meeting Report

9th International Conference on Chemometrics in Analytical Chemistry (CAC-2004), Lisbon, Portugal, 20–23 September 2004

CAC-2004 was hosted by the Center for Biological and Chemical Engineering, Technical University of Lisbon (IST). Attendance by 240 people from 40 different countries of all continents (predominantly from Europe and North America) ensured a lively and stimulating meeting, its main theme being 'New Challenges for a Maturing Science'. The program included 49 oral presentations and more than 190 posters. Detailed information about the meeting can be found on the website <http://dequim.ist.utl.pt/cac2004/program.htm>. The 49 lectures included presentations by most of the leading chemometricians and the majority of the chemometrics founding fathers. The conference was sponsored by several organizations.

José C. Menezes and Joaquim E. Silva, CAC-2004 chairmen, and their most courteous team should be congratulated and thanked for the excellent job they did, which definitely contributed to the success of this conference. The social program was eventful and gastronomically superb, from the opening reception to the conference banquet in Sintra.

The first-day sessions began and ended with the Martens family: an opening lecture by Harald on chemometrics and the new '-omics' (genomics, metabonomics, metabolomics, proteonomics) and a closing one by Magni on the '-ometrics' in the analysis of quality (chemometrics, sensometrics). This first day was devoted to biologically related problems approached by traditional as well as by novel chemometrics methods and process analysis. The challenges for chemometrics in the pharmaceutical industry were especially emphasized.

As Harald Martens pointed out, besides the usual methodological challenges arising from interdisciplinary works, there is also a considerable cultural challenge to be addressed, coming mainly from attitude and jargon barriers. Chemometricians should reach out by using a common language in order to describe and apply their methodology to the complex data generated by the '-omics' disciplines.

The day was rounded off with a talk by Bernard Vandeginste on the history, foundation and founding (grand) fathers of chemometrics. A detailed history was recounted and highlighted by a vivid presentation of the first chemometrics software ARTHUR (1975, in FORTRAN for mainframe) from Kowalski's group. A video recording by Professor Massart taped a week before CAC-2004 was shown during this presentation as a welcoming address to

CAC-2004 participants and its organizing committee, conveying an optimistic message about the future of chemometrics. The enthusiastic applause by the audience was a multivariate measure of how enjoyable this talk was.

On the second day the speakers concentrated mainly on process analytical technology (PAT), with the morning session being kicked off by Svante Wold's lecture on the role of chemometrics in PAT (originated 20 years ago by B. Kowalski). Wold confronted chemometricians with two great challenges: firstly, to work out ways to include chemometric methodology in overall risk evaluation, and, secondly, to ease communication by making chemometric 'outputs' understandable to everyone involved. Those are, in Wold's words, essential steps towards the routine use of chemometrics in PAT. New scenarios for action of chemometrics in pharmaceutical production and industry in general, in process analysis and in process monitoring were expounded in the following lectures.

During the conference banquet the winners of the 4th Elsevier Chemometrics Award were announced; this year the prize was split between Dr Karl Booksh from Arizona State University, USA and Dr Anna de Juan from the University of Barcelona, Spain.

The morning sessions of the third day were devoted to product design and optimization and the role of chemometrics in environmental data analysis. The afternoon sessions concentrated on the biomedical challenges for chemometrics, focusing mainly on its new applications in NMR spectra and image data analysis. The third day's activities closed with the announcement of the CAC-2004 best poster award, won by C. Ruckebush *et al.* from LASIR CNRS, Lilly, France, the same winner from the previous CAC meeting! After an intense day of work the visit to the Oceanarium was a relaxed activity greatly appreciated by all participants.

The last day of the conference was completely devoted to the *new* chemometric methods and approaches, beginning with experimental design and followed by new approaches for handling large data sets.

All in all, the material selected for the 14 thematic sessions formed an excellent representation of the challenges that face chemometricians nowadays from different areas, including systems biology, chemical processing, environmental, pharmaceutical and Zeus knows what else!

After thoughtful deliberation the permanent committee decided in Lisbon to follow the 15th century Portuguese navigators and head boldly towards the southern hemisphere placing for the first time a CAC conference, the 10th, on the other side of the equator, namely in Campinas, Brazil.

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