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Editorial

The field of chemometrics has changed dramatically over the past twenty years. Early chemometric papers focused on applications of the linear learning machine. Later, experimental design, sampling techniques, multivariate calibration, exploratory data analysis, quality control, laboratory management and more recently artificial intelligence techniques such as expert systems and neural networks became active areas of interest. Indeed the area of chemometrics has experienced phenomenal growth as evidenced by the large number of chemometric publications, and the existence of journals devoted exclusively to this field. Since modern instruments can routinely generate large quantities of data it is not surprising that there is a need for analysis of the data to extract the relevant information. Hence the future of chemometrics in analytical chemistry is ensured. In addition, some analytical methods owe their present popularity to developments in the field of chemometrics. Consider near-infrared spectroscopy, for example, which has been revolutionized because of partial least squares.

This special issue is devoted to the work of young chemometricians who will define the shape of the field as we enter the 21st century. In this issue, therefore, we aimed to collect their view on research lines and directions rather than specific research results. Developments in workstations and supercomputers as well as the availability of chemometric software packages (e.g. Matlab and Unscrambler) will ensure that the methodologies described in this issue will be within easy reach of most chemists. Hence, the field is poised for unprecedented growth. Neural networks, expert systems, high-resolution computer graphics, Kalman filtering, and multivariate analysis will be the new buzz words used by bench chemists in the 21st century. The interest in these techniques is due to the redundancy in data generated by hyphenated instruments which will ensure the universal adaption of so-called intelligent instruments, i.e. instruments that use chemometric methods for the design and analysis of experiments. As chemists rely more heavily on these chemometric techniques and computers for solutions to their experimental problems, chemometrics will become an integral part of their education at the undergraduate level. Thus, the seeds for a great revolution in analytical chemistry in the 21st century are being sown.

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