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Foreword

The focus of this issue is on the combination of chemical separation methods and chemometric data analysis. Based upon the work presented herein, what a powerful combination indeed, albeit with some challenges that must be overcome to gain broader applicability and acceptance by the general practitioner. The contributions in this issue are representative of this exciting research area, but by no means comprehensive.

Chemometrics has been loosely defined as "the development and use of mathematical techniques to extract useful information from data acquired through chemical analysis." In this context, chemometrics serves to render chemical separation methods more powerful for their intended purpose, which, as Giddings put it, is "to multiply the quantity of detailed information available about complex mixtures, and to enhance the quality of that information." Thus, the vision and purpose is not to apply chemometrics to make up for performing poor chemical separation methodology. Rather, the intent is to combine state-of-the-art chemical separation instrumentation and methodology synergistically with the emerging tools in the chemometrics field.

The most obvious application of chemometrics is to mathematically resolve overlapped peaks, and thus to enhance identification and quantification. Closely related to this application is the use of regression methods to quantify groups or classes of chemical compounds. Conversely, often one is interested in classification of samples or pattern recognition and fingerprinting. Additionally, one can apply chemometric methods to better understand chemical separation systems from a theoretical perspective, and to also optimize chemical separation methodology, namely, to determine the best experimental conditions to provide a desired separation. The list of current and possible applications of chemometrics with chemical separations is no doubt endless. All of these important applications must be put into the context of the data structure provided by the instrumentation and the availability of suitable chemometric software that should be designed to readily glean the desired information from the data.

Availability of user-friendly software is a key challenge that must be met in order for chemometrics to be more broadly applied and accepted as a routine tool. In particular, there is an on-going need for user-friendly software that can be efficiently applied to data obtained from higher order separation methods such as CE × CE, GC × GC or GC–MS (that provide a second order data structure in the form of a matrix), and GC × GC–time-of-flight MS (that provides a third order data structure in the form of a cube). Delivery on this challenge is being addressed by industry and academia, but should remain the number one priority. Furthermore, there is a need to continue to educate and, if necessary, convert the general practitioner to the ways of combining optimal chemical separations with mathematical separations, in order to best convert data to useful information. The main point is this, the rewards will be immense for the analyst who adopts and implements chemometrics into their chemical separation strategies.

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