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Preface

Enhancing chemical separations with chemometric data analysis

In this special issue, the focus is on adapting and refining chemometric data analysis approaches to enhance chemical separations, such as gas chromatography, liquid chromatography and capillary electrophoresis, in either one-dimensional or two-dimensional separation formats. Chemometric data analysis (or chemometrics) can be thought of as the development and use of mathematical techniques to extract useful information from data acquired through chemical analysis. Hence, combining chemometrics with chemical separation methods makes the separation methods more powerful and useful for their intended purpose, which, as J. Calvin Giddings put it is "to multiply the quantity of detailed information available about complex mixtures, and to enhance the quality of that information". Additionally, let us all keep in mind that as good analytical chemists, the purpose is not to apply chemometrics to make up for performing poor chemical separations. Indeed, one must strive to combine state-of-the-art chemical separation technology and methodology synergistically with the emerging algorithms and software in the chemometrics field to address current challenges in separation science. Based upon the contributions presented herein, chemometric data analysis is rapidly becoming immensely important to glean useful information from chemical separation data, e.g., information that may not otherwise be provided by more traditional data analysis approaches, or not provided in a sufficiently timely fashion.

One of the most widely used applications of chemometrics is to mathematically resolve overlapped peaks, enhancing identification and quantification. Regression methods to quantify groups or classes of chemical compounds are also used, especially in industrial applications. Classification of samples via pattern recognition and fingerprinting is yet another key application of chemometrics. Also, chemometric methods can be used to better understand chemical separation systems from a theoretical perspective, and to optimize chemical separation methodology. There are countless possible applications for chemometrics with chemical separations.

Many of the advances presented herein are in the realm of the expert, and there are still challenges that must be overcome to gain broader applicability and acceptance by the general practitioner. Making available 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. Many of the contributions demonstrated herein by many of the world's experts are aimed to address this issue of placing chemometric techniques into the toolbox for everyday practice. Furthermore, there is a need to continue to educate and convert the general practitioner to the ways of combining optimal chemical separations with chemometric tools, in order to optimally convert data to useful information. Indeed, the key point is that the rewards may be immense for the analyst who implements chemometrics into their chemical separation applications and studies.

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