



Preface

Chemometrics in chromatography

Since the introduction of the term chemometrics (in analogy with biometrics, econometrics, etc.), by Svante Wold four decades ago, to define “the art of extracting chemically relevant information from data produced in chemical experiments” [1], this art has evolved into a major and vigorous discipline with application in many research areas.

The Journal of Chromatography B has been following developments in chemometrics, since the second half of the seventies, when it published several articles that highlighted the importance of the emerging field of chemometrics, especially the application of pattern recognition techniques and multicomponent analysis [2,3]. Through the years, chemometrics has proved to be a powerful tool for chromatography and their range of applications continue to increase.

Nowadays, there has been a noticeable growth in the publication of articles relating to the application of chemometrics in chromatography due to the promising potential for application of multivariate techniques on the various aspects of chromatography. Current applications range from sample treatment and instrumental optimization to modeling and predictions of complex chromatographic systems and elucidation of their underlying structures.

The importance of chemometrics and chromatography and the growing volume of combined application all over the world was the driving force behind this Special Issue on Chemometrics and Chromatography. The articles selected for this Special Issue describe a wide battery of chemometrical approaches (principal component analysis, orthogonal projections of latent structures, partial least square, independent component analysis, hierarchical cluster analysis, support vector machine-recursive feature elimination, multivariate curve resolution-alternating least square, genetic algorithm, similarity analysis, soft independent modeling of class analogies, parallel factor analysis, quantitative structure–retention relationship, model design) on chromatographic data derived from a broad spectrum of samples (nutritional, pharmaceuticals, medicinal, human, animal, pesticides, flame retardants). In addition to these application articles, this Special Issue also includes some

reviews on data processing, multivariate calibration and experimental design. We believe that this Special Issue will benefit both familiar and unfamiliar practitioners as it covers both fundamental and applied aspects of chemometrics in chromatography.

We thank all the signing authors for their interest, enthusiasm and effort to complete their articles in a timely manner. We are indebted to the many reviewers for their very constructive and detailed and thoughtful comments which improved the quality of the articles. We also would like to express our most sincere gratitude and appreciation to Prof. Dimitrios Tsikas, Thematic Volume Editor, for proposing (three years ago) the publication of a Special Issue covering aspects of chemometrics and chromatography and also for his help throughout the development of this Special Issue. Finally, we thank Basil Nyaku, Journal Manager, and Patricia Massar, Content Development Manager, for their professional handling of the manuscripts throughout the review and production processes.

References

- [1] S. Wold, *Chemom. Intell. Lab. Syst.* 30 (1995) 109.
- [2] E. Jellum, *J. Chromatogr.* 143 (1977) 427.
- [3] M.L. McConnell, G. Rhodes, U. Watson, M. Novotny, *J. Chromatogr.* 162 (1979) 495.

Pedro Araujo*

National Institute of Nutrition and Seafood Research (NIFES), Bergen, Norway

Bjørn Grung

Department of Chemistry, University of Bergen, Bergen, Norway

* Corresponding author.

E-mail addresses: Pedro.Araujo@nifes.no (P. Araujo), bjorn.grung@kj.uib.no (B. Grung)

Available online 2 November 2012