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Chemometrics in Electroanalysis

Springer

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Preface of the Series Editor

Chemometrics and electrochemistry (including electroanalysis) are two independent and not directly related topics. However, chemometrics is of very high potential value for the treatment of electrochemical data. Still, only a few electrochemists and electroanalysts make use of it, probably because their attention is completely absorbed by the purely electrochemical problems, leaving not much time to study chemometrics. The application of chemometrics to electrochemistry needs people who understand both scientific fields to the same extend. I was very happy that Miquel Esteban, Cristina Ariño and José Manuel Díaz-Cruz from the University of Barcelona readily accepted my proposal to write this monograph, which is a unique contribution to the electrochemical literature. The authors are chemists who are very experienced in using chemometric methods, and they are equally experienced in electrochemistry and electroanalysis. I hope that this monograph will help to expand the application of chemometric methods in electrochemistry and electroanalysis, because this can be most beneficial for a sound interpretation of experimental data and for the validation of analytical procedures. Scientists primarily working in chemometrics may also benefit from the many examples and case studies from the area of electrochemistry.

Greifswald, Germany
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Fritz Scholz

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We thank our old colleague Romà Tauler, a recognized pioneer in the development and application of soft modelling techniques, for introducing us in the exciting field of MCR-ALS and to help us to apply such a powerful tool to electroanalytical data, in a time (the 1990s) dominated by hard modelling. We also thank him for his cooperation and support along the years, and for the frequent and valuable scientific discussions on the application of chemometrics to electroanalysis. In the initial years of our exploration of MCR-ALS, it was also essential the work by Jesús Mendieta and Silvia Díaz-Cruz with metallothioneins and related compounds, which settled some key aspects such as the shape constraint or the concept of electrochemical component that would be essential in all our further investigations. This acknowledgement is extended to our 'chemometrician' colleagues, Anna de Juan and Marcel Maeder, for their valuable assessment.

We also thank Núria Serrano, the youngest staff member of our research team, who has recently introduced us in the field of modified screen-printed devices, sensor arrays and electronic tongues, closely related to chemometrics. In these efforts, it has been crucial the mastery and support of Manel del Valle, which is gratefully acknowledged.

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Abbreviations

a.u.	Arbitrary units
AdSV	Adsorptive stripping voltammetry
AI	Artificial intelligence
ALS	Alternating least squares (algorithm)
ANN	Artificial neural network
ANOVA	Analysis of variance
ASV	Anodic stripping voltammetry
AWLS	Automatic weighted least squares (baseline correction)
BBD	Box–Behnken design
CCD	Central composite design
CLS	Classical least squares (calibration)
CV	Cyclic voltammetry
DD	Doehlert design
DF	Discriminant function
DPP	Differential pulse polarography
DPV	Differential pulse voltammetry
DWT	Discrete wavelet transform
EFA	Evolving factor analysis
ER	Model error rate
FFT	Fast Fourier transform
GPA	Gaussian peak adjustment
GSAM	Generalized standard addition method
GUI	Graphical user interface
ICP-MS	Inductively coupled plasma with mass spectrometry detection
ICP-OES	Inductively coupled plasma with optical detection
ILS	Inverse least squares (calibration), also known as MLR
IQR	Interquartile range
KES	Knowledge engineering system
LC-MS	Liquid chromatography with mass spectrometry detection
LDA	Linear discriminant analysis

LOD	Limit of detection
lof	Lack of fit
LOQ	Limit of quantification
LSW	Linear sweep voltammetry
LV	Latent variable
MCR	Multivariate curve resolution
MCR-ALS	Multivariate curve resolution by alternating least squares
MLR	Multiple linear regression (calibration), also known as ILS
MSC	Multiplicative scatter correction
MT	Metallothioneins
NER	Model non-error rate
NIPALS	Non-linear iterative partial least squares (algorithm)
NIR	Near infrared (spectroscopy)
NMR	Nuclear magnetic resonance
NPLS	Multidimensional partial least squares
OVAT	(Changing) one variable at a time
PARAFAC	Parallel factor analysis
PC	Principal component; phytochelatin
PCA	Principal component analysis
PCR	Principal component regression (calibration)
PLS	Partial least squares (calibration)
PLS-DA	Partial least squares discriminant analysis
PRESS	Predicted residual error sum of squares
RE	Relative error
RMSEC	Root mean square error of calibration
RMSECV	Root mean square error of cross validation
RMSEP	Root mean square error of prediction
RSD	Relative standard deviation
SIMPLISMA	Simple-to-use interactive self-modelling mixture analysis
SV	Stripping voltammetry
SVD	Singular value decomposition
SVM	Support vector machine
SWV	Square-wave voltammetry
VIP	Variable importance in projection