



# Chemometrics and electrochemistry: a useful tandem to be shown to university students

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## Abstract

A short discussion is given of the convenience of integrating electrochemistry and chemometrics in university degrees related to chemistry, and some selected examples are presented to illustrate the possibilities of combining both disciplines for solving (electro)chemical problems of different nature.

## Introduction

Chemometrics can be defined as “the chemical discipline that uses mathematical and statistical methods, (a) to design or select optimal measurement procedures and experiments, and (b) to provide maximum chemical information by analyzing chemical data” [1]. The term chemometrics was introduced in 1972 by Svante Wold, professor of Organic Chemistry at Umeå University, Sweden, and Bruce R. Kowalski, professor of Analytical Chemistry at University of Washington, Seattle, USA. In chemistry, it is similar to the previous *econometrics* and *biometrics* terms for economic and biological sciences, respectively.

The foundation of the International Chemometrics Society in 1974 has led to the first description of this discipline. In the following years, some journals devoted special sections to papers on chemometrics (Analytical Chemistry, *Analitica Chimica Acta*, *Talanta*, *Applied Spectroscopy*, ...). In the 1980s, new journals were founded to cover this field: *Journal of Chemometrics* (Wiley), *Chemometrics and Intelligent Laboratory Systems* (Elsevier), and *Journal of Chemical Information and Modeling* (ACS publications).

Several important books/monographs on chemometrics were also first published in the 1980s, including the first edition of Malinowski and Howery's *Factor Analysis in Chemistry* [2], Sharaf et al.'s *Chemometrics* [3]; Massart et al. *Chemometrics:*

a textbook [4]; and *Multivariate Calibration* by Martens and Naes [5]. More recently, a reference work (in 4 volumes) has been published (two editions at the moment) [6].

Nowadays, even with the contribution of many authors in recent years, application of chemometrics to electrochemistry, in general, and electroanalytical chemistry, in particular, is still relatively scarce as compared with what happens in spectroscopy and, more recently, in image analysis. We guess this is the consequence of the intimate link between mathematics and electrochemistry, where the essential body of knowledge concerns: (i) proper physico-chemical pictures of the electrochemical processes and the corresponding joint transport phenomena, (ii) the analytical or numerical solutions of these mathematical formulations (outlined according to the corresponding models), and hopefully (iii) the proper physico-chemical interpretation of the electroanalytical data. This approach is usually designated as *hard modeling*, and it is the common approach used in electrochemical investigations and found in literature. However, in many cases, the postulation of a theoretical physico-chemical model is very difficult because the electrode process (including accompanying chemical reactions), the transport phenomena process, or both of them are rather involved. In such cases, the lack of a hard model makes of the highest interest whatever another type of approach.

The global alternative approach can come from chemometrics, and it is based on extracting results and/or identify models from numerical and statistical analysis of the data, instead of fitting an assumed a priori theoretical model to the experimental data. This new approach is denoted as *soft-modeling* to distinguish it clearly from the classical approach [11–13].

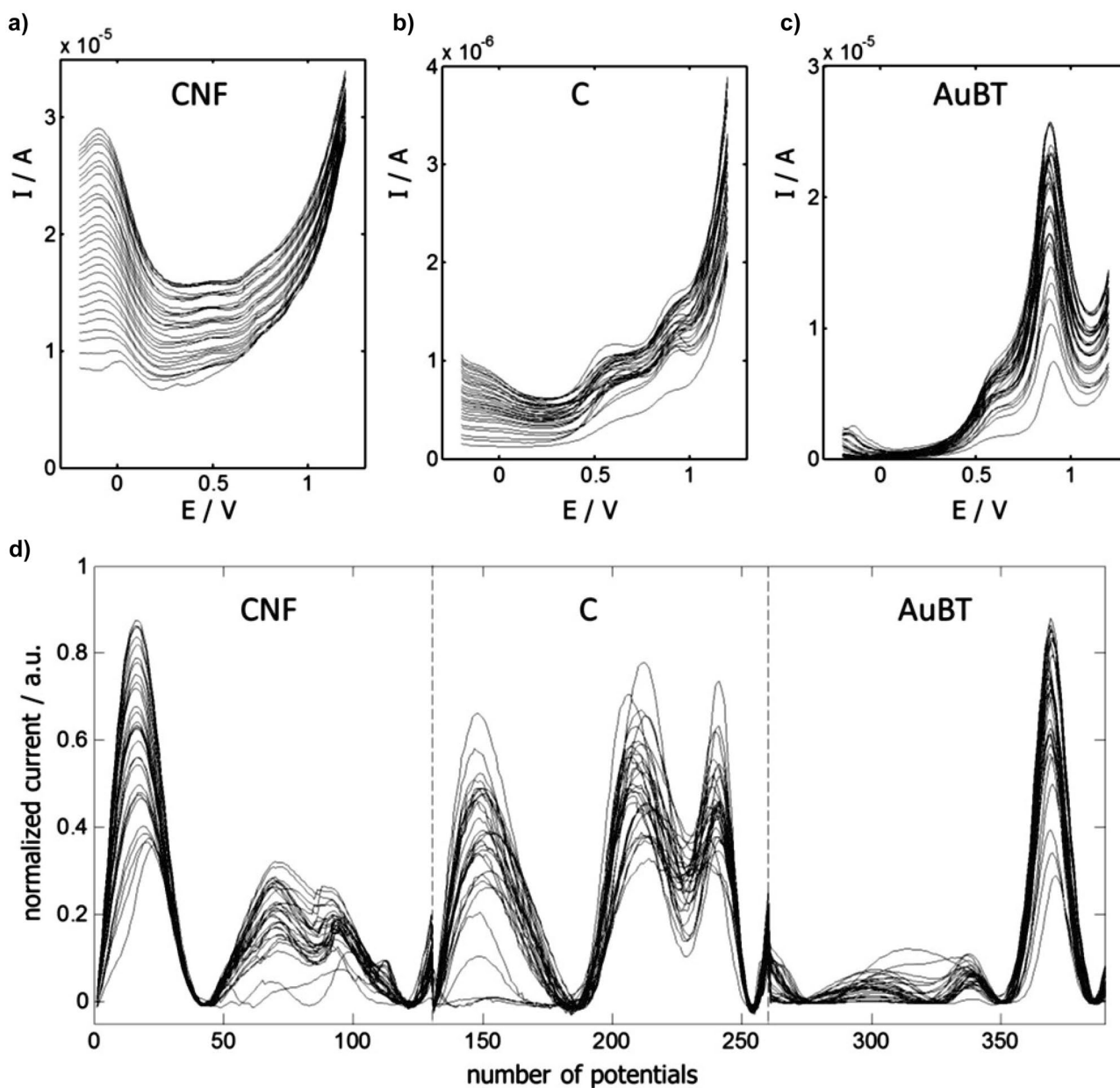
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Nowadays, chemometrics is applied in the field of electroanalysis for different purposes: experimental design, signal processing, exploratory data analysis, and, especially, calibration [11, 13, 14]. Methods intended for the evaluation of linear data such as principal component analysis (PCA) or partial least squares (PLS) calibration can be applied to many electrochemical data, provided that a few additional components can account for slight deviations from linearity. In the most

extreme situations, non-linear methods such as artificial neural networks (ANN) or support vector machine (SVM) can be an alternative. But, independently of the chemometric method employed, it must be emphasized that the inherent characteristics of electroanalytical data must be considered for a sound interpretation of the results.

As compared to spectra, electroanalytical signals have clear drawbacks, as the poorer reproducibility, their strong



**Fig. 1** Differential pulse voltammograms (DPV) obtained from mixtures of cysteine (Cys), homocysteine (hCys), and glutathione (GSH) with an electronic tongue integrated by three commercial screen-printed electrodes of carbon nanofibers, CNF **a**, carbon, C **b** and gold cured at low temperature, AuBT **c**. In **d**, it is shown the augmented data matrix, row-wise constructed with the voltammograms of indi-

vidual sensors **a–c** previously baseline-corrected and normalized. The analysis of pure solutions of the amino thiols shows that their oxidation signals appear at increasing peak potentials in the order Cys, hCys, and GSH, and this is the order of the peaks (from left to right) observed in the graphs of the mixtures. Reproduced from [15] with permission

dependence on measuring parameters, the matrix effects or the usual deviations from linearity, but they also have advantages, like the well-defined shape (peaks and sigmoids that can be easily adjusted by parametric functions). Anyway, some of the most recent analytical applications of the electrochemical techniques and methods are intimately related to chemometric methods, and their development would not be possible without chemometrics.

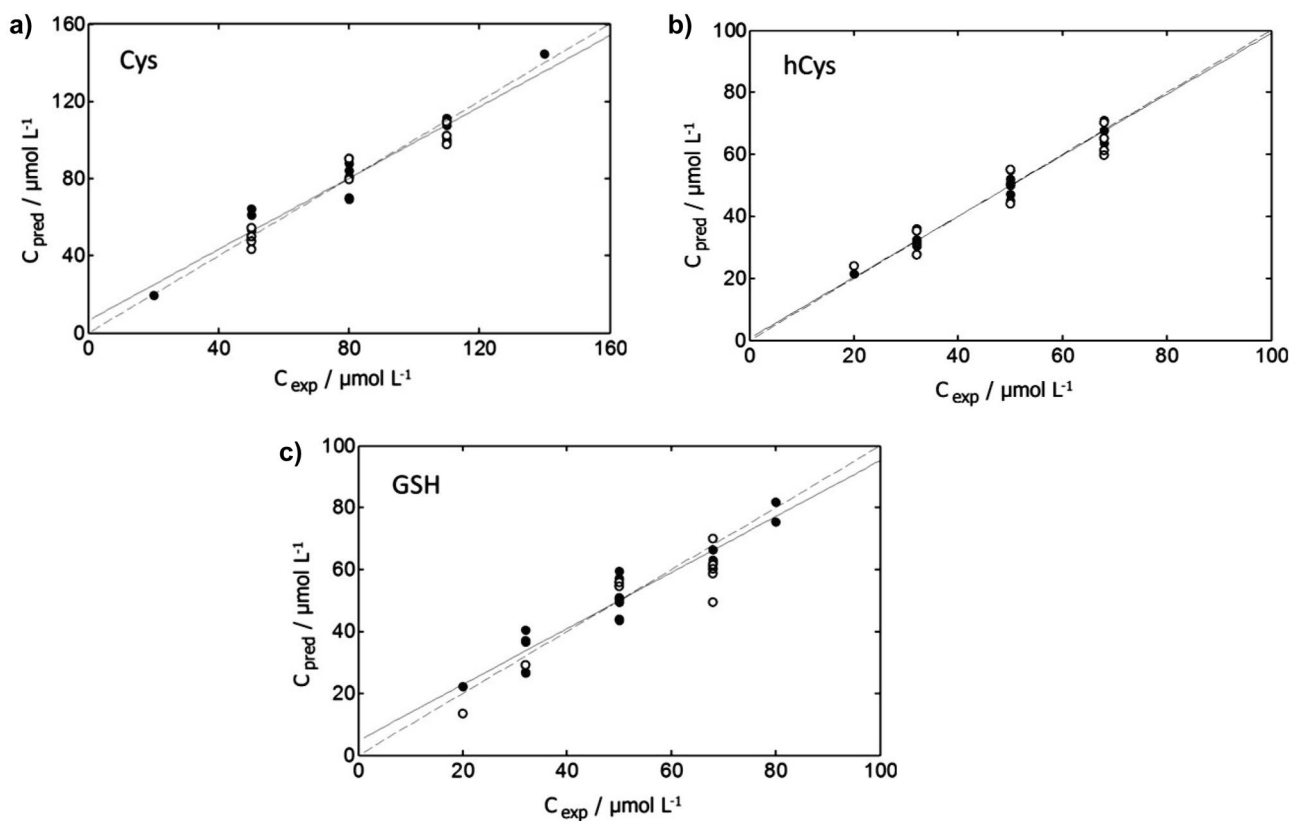
## University teaching of chemometrics and electrochemistry

In the departments/faculties of chemistry, the teaching of chemometrics is usually under the responsibility of the analytical chemistry unit/section/department. Thus, in practice, it is more related to the foundations of analytical chemistry and instrumental analysis, especially the optical techniques, than to other subdisciplines as, for instance, electrochemistry. Because of that, chemometrics is usually not mentioned in the courses of electrochemistry.

Chemometrics has dedicated subjects in many Spanish universities at both Degree and M.Sci. levels, usually as an optional subject. This is the case of the Degree of Chemistry

at the University of Barcelona, where there is the optional subject “chemometrics” of 3 ECTS, which is among the most appreciated by the students in the surveys. Half of its time (15 h) is devoted to theory class introducing the fundamentals of the most usual chemometric techniques: principal component analysis (PCA), principal component regression (PCR), partial least squares (PLS), soft independent modeling of class analogy (SIMCA), and partial least squares discriminant analysis (PLS-DA). The other half of the time (6 sessions of 2 h) is carried out in the computer classroom applying the techniques above to numerical examples. For this purpose, the commercial software PLS-Toolbox [7], by Eigenvector Research, is used. This is a Matlab-based [8] toolbox with a really user-friendly interface. PLS\_Toolbox can operate in the same way as other Matlab toolboxes or compiled together with Matlab into a compact version named SOLO. Besides the computer sessions, the students work in groups using their own computers to deal with more complex sets of data. Although most of the examples are from spectroscopic origin, in the last years, some electrochemical data have also been introduced.

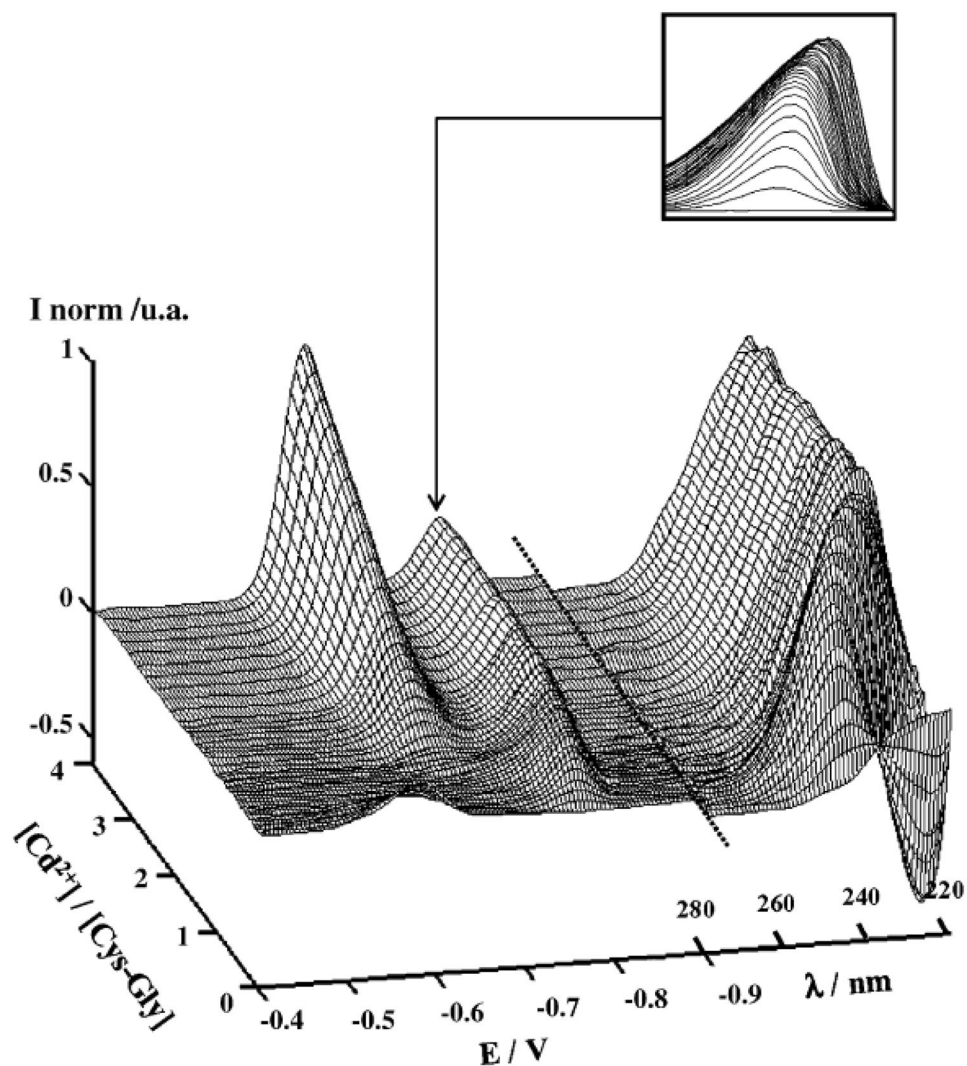
In the following, we will describe very briefly some applications published by our research team that can be mentioned when teaching electrochemistry or electroanalysis to



**Fig. 2** Predicted versus experimental concentrations of cysteine **a**, homocysteine **b**, and glutathione **c** obtained with three individual PLS-1 models adjusted to the data shown in Fig. 1d. Calibration and

external validation values are denoted with solid and empty circles, respectively. Reproduced from [15] with permission

**Fig. 3** Augmented data matrix containing normalized DP voltammograms and CD spectra measured at different ratios of  $\text{Cd}^{2+}$  and the peptide Cys-Gly at pH 7.5 in the presence of  $\text{KNO}_3$   $0.01 \text{ mol L}^{-1}$  and PIPES buffer  $1 \cdot 10^{-3} \text{ mol L}^{-1}$ . Reproduced from [17] with permission



illustrate for the students the convenience of a sound knowledge of chemometrics to extract a maximum of information from electrochemical data.

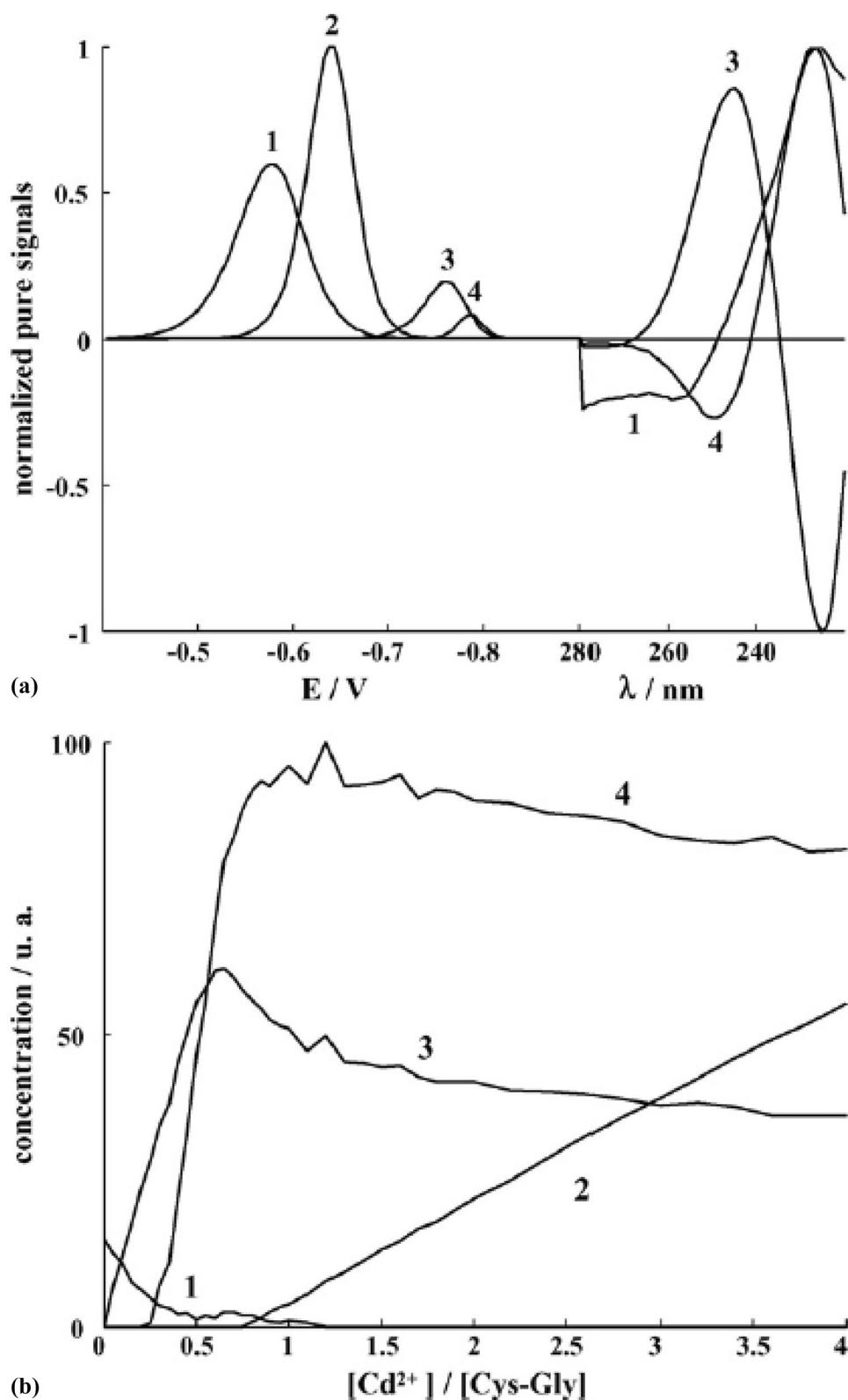
## Selected applications

The first application is the use of a voltammetric electronic tongue for the quantification of amino thiols [15]. Electronic tongues are arrays of sensors having insufficient selectivity to work stand-alone in the determination of one or more analytes [16]. However, if they have cross-response towards a group of analytes, they can be grouped into an electronic tongue. Cross-response means mixed sensitivity (understanding sensitivity as the slope of the calibration plot). For instance, sensor 1 has sensitivities of 10 and 30 towards analytes A and B, respectively, whereas sensor 2 has sensitivities of 40 and 25 towards the same analytes).

In the example of ref. [15], we have three sensors based on commercial screen-printed electrodes (SPE) of different composition: carbon nanofibers (CNF), carbon (C), and gold cured at low temperature (AuBT). Figure 1a-c show the differential pulse voltammograms (DPV) obtained for different mixtures of three amino thiols: cysteine (Cys), homocysteine (hCys), and glutathione (GSH). These individual voltammograms are not able to distinguish among all three substances. However, the combination of these data into a row-wise augmented matrix, after a preliminary baseline correction and normalization (Fig. 1d), improves the overall selectivity. Then, the application of three individual partial least squares (PLS-1) calibration models allows a reasonable quantification of all three amino thiols, as shown by Fig. 2.

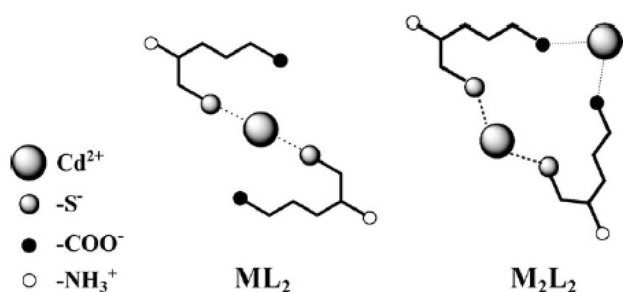
The second example is the application of multivariate curve resolution by alternating least squares (MCR-ALS) to a set of differential pulse (DP) voltammograms and circular dichroism (CD) data obtained for the system

**Fig. 4** Normalized pure signals (voltammograms and spectra) **a** and concentration profiles **b** obtained for the different species involved in the binding of  $\text{Cd}^{2+}$  by the peptide Cys-Gly. The species are Cys-Gly (1),  $\text{Cd}^{2+}$ -ion (2),  $\text{Cd}(\text{Cys-Gly})_2$  (3), and  $\text{Cd}_2(\text{Cys-Gly})_2$  (4). Reproduced from [17] with permission



$\text{Cd}^{2+}$ —Cys-Gly peptide. The augmented data matrix is shown in Fig. 3. The application of MCR-ALS with a set of restrictions imposed to keep the physico-chemical meaning

of the solution produces the pure signals (Fig. 4a) and the concentration profiles (Fig. 4b) of the different substances involved in the complexation equilibria. This information

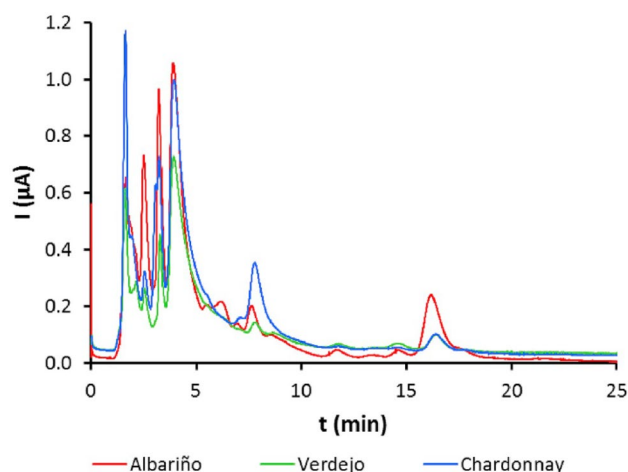


**Fig. 5** Proposed structures for the complexes on the basis of the results shown in Fig. 4. Reproduced from [17] with permission

allows one to propose binding mechanisms such as this shown in Fig. 5.

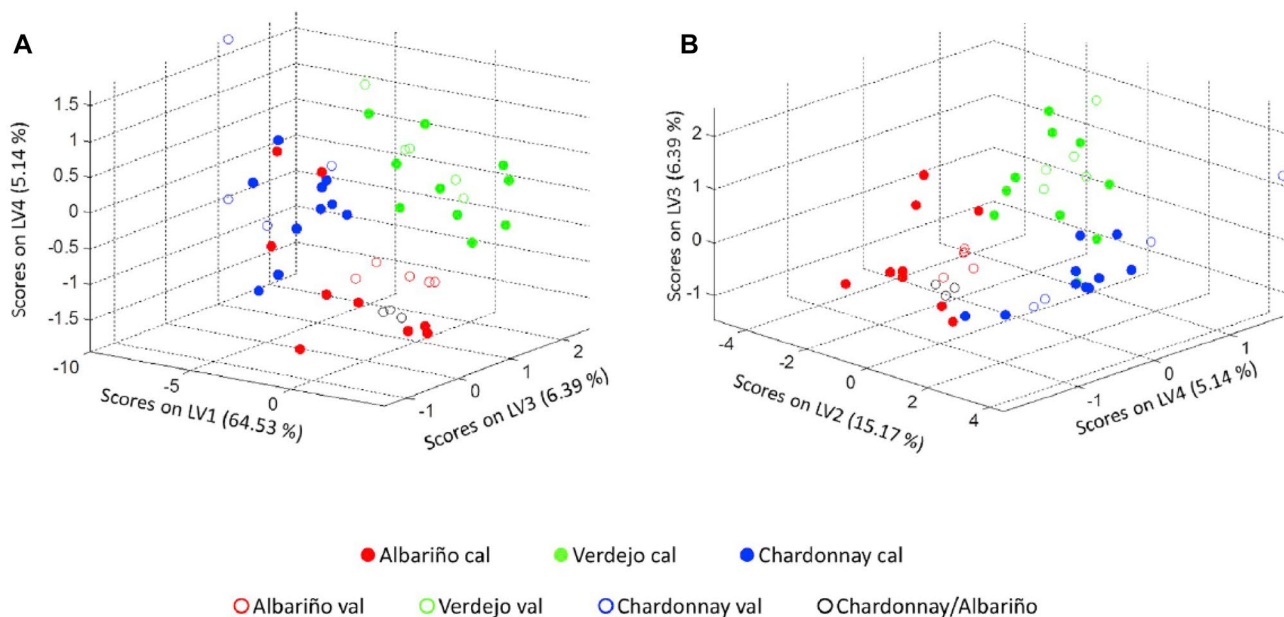
The third example is the use of liquid chromatography (HPLC) with amperometric detection (AD) to discriminate among three varieties of white wine (Albariño, Verdejo, and Chardonnay). This is a typical case of chromatographic fingerprinting for the discrimination of samples, but with the electrochemical view in the detection. Figure 6 shows typical chromatograms of the three wine varieties, which do not have a characteristic compound to discriminate them, but a characteristic pattern of the multiple peaks conforming the chromatographic profile in this selected time window of 25 min.

In this work, wine samples were distributed among a calibration set (4 Albariño, 4 Verdejo, and 4 Chardonnay) and a validation set (2 Albariño, 2 Verdejo, 2 Chardonnay, and



**Fig. 6** Typical HPLC-AD chromatograms of the three wine varieties considered (Albariño, Verdejo, and Chardonnay) using a SeQuant ZIC-pHILIC column with a mobile phase of 0.05% (v/v) TFA: ACN (19:81) and a flow rate of 1 mL min<sup>-1</sup>. AD was carried out with a screen-printed gold electrode at a fixed potential of +1.00 V vs. Ag/AgCl (3 mol L<sup>-1</sup> KCl) reference electrode. Reproduced from [18] with permission

1 Albariño/Chardonnay), and a PLS-DA model was built. The resulting 3D scores plot is shown in Fig. 7. In the plot of Fig. 7a (latent variables LV1, LV3, and LV4), Verdejo samples can be easily distinguished, whereas in the plot of Fig. 7b (with LV2, LV3, and LV4) allows the discrimination between Albariño and Chardonnay samples.



**Fig. 7** 3D-scores plots obtained after PLS-DA models built from white wine HPLC-AD signals. Latent variables 1, 3, and 4 **A** or 2, 3, and 4 **B** are considered. Calibration (cal) and validation (val) sets are

represented by filled and empty symbols, respectively. Reproduced from [18] with permission

## Conclusions

Electrochemists cannot restrict their data management strategies to the combination of deterministic equations about (electro)chemical equilibrium, adsorption, kinetics, and mass transport. Contemporary science and technology are exploring systems of increasing complexity and generating huge amounts of data coming from different measuring devices. Fortunately, electrochemical sensors are an important part of such devices and chemometric tools can be very useful to extract the valuable information hidden there. This is why we believe that at the university level, the courses of electrochemistry should incorporate some chemometric contents and the courses on chemometrics should include some examples of the multivariate analysis of electrochemical data.

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## References

- Otto M (2007) Chemometrics. WILEY-VCH Verlag, Weinheim (ISBN-10: 9783527314188, ISBN-13: 978-3527314188)
- Malinowski ER, Howery DG (1980) Factor analysis in chemistry. Wiley, New York (other editions followed in 1989, 1991 and 2002; ISBN 978-0471058816)
- Sharaf MA, Illman DL, Kowalski BR (1986) Chemometrics. Wiley, New York (ISBN 978-0-471-83106-8)
- Massart DL, Vandeginste BGM, Deming SM, Michotte Y, Kaufman L (1988) Chemometrics: a textbook. Elsevier, Amsterdam (ISBN 978-0080868295)
- Martens H, Naes T (1989) Multivariate calibration. Wiley, New York (ISBN 978-0-471-93047-1)
- Brown S, Tauler R, Walczak B (2020) Comprehensive chemometrics: chemical and biochemical data analysis, 2nd edn. Elsevier, Amsterdam (ISBN 978-0444641663)
- PLS\_Toolbox, Eigenvector Research, Inc, Version 8.9.2, 2021. Manson, WA USA. <https://eigenvector.com/software/pls-toolbox/>
- Matlab, Mathworks Inc, Version R2021b, 2021. Natick, MA, USA. <https://es.mathworks.com/products/matlab.html>

- Brown SD, Bear RS Jr (1993) Crit Rev Anal Chem 24:99–131. <https://doi.org/10.1080/10408349308048820>
- Richards E, Bessant C, Saini S (2002) Electroanalysis 14:1533–1542. [https://doi.org/10.1002/1521-4109\(200211\)14:22%3c1533::AID-ELAN1533%3e3.0.CO;2-T](https://doi.org/10.1002/1521-4109(200211)14:22%3c1533::AID-ELAN1533%3e3.0.CO;2-T)
- Esteban M, Ariño C, Díaz-Cruz JM (2006) Trends Anal Chem 25:86–92. <https://doi.org/10.1016/j.trac.2005.07.009>
- Ni Y, Kokot S (2008) Anal Chim Acta 626:130–146. <https://doi.org/10.1016/j.aca.2008.08.009>
- Díaz-Cruz JM, Esteban M, Ariño C (2019) Chemometrics in electroanalysis. In: Scholz F (ed) Monographs in electrochemistry. Springer Nature, Cham, Switzerland (ISBN 978-3030213862)
- Esteban M, Ariño C, Díaz-Cruz JM (2020) Chemometrics in electrochemistry. In: Brown S, Tauler R, Walczak B (eds) Comprehensive chemometrics: chemical and biochemical data analysis, 2nd edn. Elsevier, Oxford (ISBN 978-0444641656)
- Pérez-Ràfols C, Gómez A, Serrano N, Díaz-Cruz JM, Ariño C, Esteban M (2017) Electroanalysis 29:1559–1565. <https://doi.org/10.1002/elan.201700053>
- del Valle M (2010) Electroanalysis 22:1539–1555. <https://doi.org/10.1002/elan.201000013>
- Alberich A, Ariño C, Díaz-Cruz JM, Esteban M (2007) Anal Chim Acta 584:403–409. <https://doi.org/10.1016/j.aca.2006.11.063>
- Pérez-Ràfols C, Subirats X, Serrano N, Díaz-Cruz JM (2019) Talanta 201:104–110. <https://doi.org/10.1016/j.talanta.2019.03.099>

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in the Autonomous University of Barcelona (Spain). She was appointed Associate Professor in 2016. She has participated in 13 competitive research projects (4 as PI), has supervised 2 Ph.D. Theses plus 3 more currently in progress and 30 Degree and M.Sci. Theses, and has collaborated with many Spanish and foreign research groups. This has generated 81 indexed publications (55 in Q1), with 1702 citations and h-index 24 (SCOPUS), and several book chapters. She has participated in 54 conferences with 91 communications. She has registered a Spanish patent that is in commercial exploitation. She belongs to the Editorial Board of Chemosensors and has been guest editor of special issues of Sensors (4), Chemosensors (2) and 1 topic shared between Biosensors, Sensors and Chemosensors. She has been evaluator of scientific projects

for funding agencies in the Czech Republic, France, El Salvador and Chile. Their research contributions are inside the fields of electroanalysis, environment, chemometrics and food science.



**José Manuel Díaz-Cruz** is Full Professor of the Department of Chemical Engineering and Analytical Chemistry at the University of Barcelona (UB) and member of the Electroanalysis Group since 1988. Following studies of Chemistry at UB, he graduated in 1988 and obtained the Ph.D. degree in 1992, also at UB. In 1990–91 and 1993 he worked for 16 months in the University of Wageningen (The Netherlands). He was appointed Associate Professor in 1995 and Full Professor in 2019 and was Secretary (2001–

03) and Vice-Dean (2003–04) of the Faculty of Chemistry of UB. Since 2022 he is a member of the Governing Board of the Water Research Institute of UB. He has joined 24 competitive research projects (2 as PI), has supervised 9 Ph.D. Theses and more than 30 Degree and M.Sci. Theses and has collaborated with many international research groups. This has produced 132 contributions to congresses, a book, 10 book chapters and 170 indexed publications (120 in Q1), with 3600 citations and h-index 32 (SCOPUS). He has been reviewer for many scientific journals and research agencies of Spain and Chile, has guest-edited issues of 'Sensors' and 'J. Food Quality' and belongs to the Editorial Board of 'Sensors'. He has registered a patent and a license contract still in exploitation. Their research contributions have been focused on analytical chemistry, electroanalysis, chemometrics, sensors, environment and food science.



**Cristina Ariño** is Full Professor of the Department of Chemical Engineering and Analytical Chemistry at the University of Barcelona (UB), Spain. Following studies of Chemistry at UB, she obtained the Ph.D. degree in 1986 and was appointed Associate Professor in 1987 and Full Professor in 2020. She has participated in more than 20 competitive research projects, has supervised 8 Ph.D. Theses, has registered a Spanish patent that is in commercial exploitation and has published more than 140 research

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**Miquel Esteban** is Full Professor (1993), Secretary and former Head of the Department of Chemical Engineering and Analytical Chemistry at the University of Barcelona (UB) and cofounder of the Electroanalysis Group at 1980. Graduated in Chemistry (1977) and PhD (1984) at UB. In 1986-87 he worked (10 months) in KFA-Jülich (Germany) and Wageningen University (Netherlands). In 1994 and 1997 Invited Researcher (8 months) at JRC-IRMM at Geel (Belgium). He has recognized 7 research six-year term,

has participated in ca. 25 competitive research projects, many of them as PI, supervised 5 PhD Theses and a high number of Degree and MSc Theses. This has generated more than 200 publications, with 4389 citations and h-index 34 (SCOPUS). He is co-author of the book *Chemometrics in Electroanalysis* (Springer, 2019) and some book chapters, one of them inside the Elseviers Reference Work *Comprehensive Chemometrics* (1st Ed. 2009; 2nd Ed. 2020). He has registered a Spanish patent and a license contract still in exploitation. His research has been focused on electroanalysis, chemometrics, sensors, environment and food science. He has been Coordinator in several editions of the Erasmus-Mundus Master in Quality in Analytical Laboratories (EMQAL).