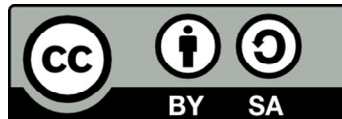




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BARCELONA

Multivariate Signal Processing for Quantitative and Qualitative Analysis of Ion Mobility Spectrometry data, applied to Biomedical Applications and Food Related Applications

Ana Verónica Guamán Novillo



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**Multivariate Signal Processing for Quantitative and
Qualitative Analysis of Ion Mobility Spectrometry
data, applied to Biomedical Applications and Food
Related Applications**

by

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“Si caminas solo irás más rápido; si caminas acompañado llegarás más lejos” – proverbio chino.

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ABSTRACT

The emerging growth in the use of Volatile Organic Compounds (VOC) for screening and monitoring substances has brought a development of new analytical techniques. There are several applications where the measurement of VOC results to be useful, such as: toxic leaks, air quality measurements, explosive detection, monitoring of food and beverages quality, diagnosis of diseases, etc. Some of this applications claim for fast responses or even real time responses. In this context, there are few analytical techniques for performing gas phase analysis, among of them Ion Mobility Spectrometry (IMS).

IMS is a fast analytical device based on the time of flight of ions in a drift tube. The response of IMS lasts typically few seconds, but it can be even less than a second. This fast response has drifted its use towards novel applications, such as biomedical and food applications (bio-related applications). Nonetheless, it has also brought the need to analyze complex spectra with hundreds of compounds. In fact, tackling this disadvantage is the main focus of this thesis, where new algorithms for enhancing the IMS performance are investigated when are applied to bio-related applications.

Nonlinear behavior and charge competitions of IMS responses are important issues that need to be addressed. Both effects have a direct impact in the IMS spectra interpretation –especially when real dataset are studied. Additionally, the use of univariate spectra analysis, where peaks information is extracted manually, becomes unfeasible in bio-related applications. In this context, this work introduces multivariate methodologies focused on quantitative and qualitative analysis.

In the case of quantitative analysis, calibration models were built using univariate methodology, Partial Least Squares (PLS) and Multivariate Curve Resolution techniques (MCR). The quantitative analysis aims tackling the main issues of IMS such as non linearities and mixture effect. Definitely, univariate techniques provides poor or overoptimistic results that minimize the impact of the IMS use. The results show a really improvement on the performance when multivariate techniques were used. Regarding the results between MCR and PLS, the main difference is the interpretability that offers MCR.

In the case of qualitative analysis, two different approaches were planned for building models for classes' discrimination. The first approach consisted on building a model through principal component analysis and linear discriminant analysis, besides of using robust cross validation methodology for obtaining reliable results. This methodology were implemented in samples of wine, where main motivation was found discrimination regarding to their origin. The results were fully satisfactory because the model was able to separate four groups with a high accuracy rate. The second approach involves the use of Multivariate Curve Resolution – Lasso algorithm for extracting pure components of samples from rats' breath and then use a feature selection technique for obtaining the most representative features subset. In this case, the objective of the application was to find a model that discriminate rats with sepsis from control rats. The results shows there were few pure components of IMS that generate a discriminatory model that means there are specific compounds in the breath linked with the disease.

Summarizing, the following proposal has as main objective resolving open issues in stand-alone IMS that are applied to the analysis of bio-related applications. Two major investigation lines were proposed in this thesis: (i) qualitative analysis and (ii) quantitative analysis. The qualitative analysis covers pre-processing algorithms and the developing of new methodologies for building models in bio-related applications. The quantitative analysis are focused on highlighting the importance of the use of multivariate techniques instead of univariate techniques. In order to reach the objectives of this thesis, a set of datasets were created, which are detailed on the content of this thesis. The results and main conclusions are deeply explained in the extended proposal.

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