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PII: S0584-8547(17)30354-3
DOI: doi:10.1016/j.sab.2018.03.007
Reference: SAB 5395

To appear in: *Spectrochimica Acta Part B: Atomic Spectroscopy*

Received date: 5 August 2017
Revised date: 4 March 2018
Accepted date: 14 March 2018

Please cite this article as: A. Safi, B. Campanella, E. Grifoni, S. Legnaioli, G. Lorenzetti, S. Pagnotta, F. Poggialini, L. Ripoll-Seguer, M. Hidalgo, V. Palleschi , Multivariate calibration in Laser-Induced Breakdown Spectroscopy quantitative analysis: The dangers of a 'black box' approach and how to avoid them. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Sab(2017), doi:10.1016/j.sab.2018.03.007

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Multivariate calibration in Laser-Induced Breakdown Spectroscopy quantitative analysis: the dangers of a 'black box' approach and how to avoid them

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Abstract

The introduction of multivariate calibration curve approach in Laser-Induced Breakdown Spectroscopy (LIBS) quantitative analysis has led to a general improvement of the LIBS analytical performances, since a multivariate approach allows to exploit the redundancy of elemental information that are typically present in a LIBS spectrum. Software packages implementing multivariate methods are available in the most diffused commercial and open source analytical programs; in most of the cases, the multivariate algorithms are robust against noise and operate in unsupervised mode. The reverse of the coin of the availability and ease of use of such packages is the (perceived) difficulty in assessing the reliability of the results obtained which often leads to the consideration of the multivariate algorithms as 'black boxes' whose inner mechanism is supposed to remain hidden to the user. In this paper, we will discuss the dangers of a 'black box' approach in LIBS multivariate analysis, and will discuss how to overcome them using the chemical-physical knowledge that is at the base of any LIBS quantitative analysis.

Keywords: LIBS; Cast Iron; Calibration Curves, Partial Least Squares Analysis; Artificial Neural Networks

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