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Critical Aspects of Data Analysis for Quantification in Laser-Induced Breakdown Spectroscopy

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Abstract

In this study, a collaborative contest focused on LIBS data processing has been conducted in an original way since the participants did not share the same samples to be analyzed on their own LIBS experiments but a set of LIBS spectra obtained from one single experiment. Each participant was asked to provide the predicted concentrations of several elements for two glass samples. The analytical contest revealed a wide diversity of results among participants, even when the same spectral lines were considered for the analysis. Then, a parametric study was conducted to investigate the influence of each step during the data processing. This study was based on several analytical figures of merit such as the determination coefficient, uncertainty, limit of quantification and prediction ability (i.e., trueness). Then, it was possible to interpret the results provided by the participants, emphasizing the fact that the type of data extraction, baseline modeling as well as the calibration model play key roles in the quantification performance of the technique. This work

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