SciAps ApNotes
November 2026



Developing Quantitative LIBS Calibrations

with the SciAps Z-903

An independent research study demonstrates a chemometrics-assisted approach to quantitative elemental analysis using broadband handheld LIBS.

Introduction

Handheld laser-induced breakdown spectroscopy (LIBS) enables rapid elemental analysis in the field. However, moving from identifying elements to reliably quantifying their concentrations requires a well-designed calibration. An independent study published in Applied Sciences in 2025 demonstrates how reference materials and multivariate data analysis can be combined to develop quantitative calibrations for the SciAps Z-903.

Calibration Method

Researchers developed a calibration for major, minor, and trace elements in silica-based archaeological materials using **17 reference samples**: eight certified reference materials (CRMs) and nine geological samples with independently established chemical compositions.

The workflow combined several key steps:

- **Reference materials:** Samples with known compositions provided the basis for calibration and evaluation.
- **Spectral preprocessing:** Baseline correction and Standard Normal Variate (SNV) normalization helped prepare the spectra for modeling.
- **Multivariate calibration:** Partial Least Squares (PLS) regression related spectral information to known elemental concentrations.
- **Variable selection:** Variable Importance in Projection (VIP) helped identify spectral variables contributing to the predictive models.
- **Model validation:** Calibration, cross-validation, and validation results were evaluated to assess predictive performance.

This approach uses information across the broadband spectrum rather than relying solely on individual emission lines, helping researchers account for the complexity of multi-element samples.



Above: Archaeological samples collected from the Archaeological Park of Tindari (Italy), providing a reference for (F): front side, (B): back side. All Specimens are shown at the same scale. See original study for exact dimensions.

Below: Number of replicates collected for each investigated archaeological sample.

Sample Name	Material	Replicates
TY_MA_7	Colorless glass	1
TY_MA_8	Green glass	1
TY_MA_9	Green glass	3
TY_MA_15	Glass	3
TY_MA_20	Glass	3
TY_MA_51	Obsidian	2
TY_MA_52	Volcanic rock	7
TY_OU_14	Brick	1
TY_OU_15	Brick	1

Results & Discussion

The researchers developed quantitative models for 19 elements, including Na, Mg, Al, Si, K, Ca, Fe, Cu, Zn, and Pb. They then applied the calibration to nine archaeological samples, including ancient glass, bricks, volcanic rock, and obsidian from the Archaeological Park of Tindari in Sicily, Italy.

The composition of the obsidian and millstone samples suggested similarities to volcanic materials from the nearby Aeolian Islands.

The glass samples showed elemental profiles consistent with Roman-era glass artifacts found elsewhere in Sicily, supporting a production technology involving natron as a flux, lime as a stabilizer, and calcareous sands as a raw material.

The two brick samples showed somewhat different elemental profiles, potentially reflecting differences in production techniques. The researchers appropriately noted that additional analyses would be required for definitive classification.

Practical Workflow

The research highlights an important distinction between having access to a LIBS spectrum and extracting reliable quantitative information from that spectrum.

For quantitative applications, calibration is not simply a matter of collecting more spectra. The quality and representativeness of the reference materials, sample preparation, spectral preprocessing, statistical model, validation strategy, and measurement conditions all influence the final result.

This study provides a practical example of that workflow:

Known standards
↓
LIBS spectral acquisition
↓
Baseline correction & normalization
↓
Calibration/validation dataset selection
↓
PLS regression
↓
VIP variable selection
↓
Independent validation
↓
Quantitative elemental prediction

Conclusion

The independent research demonstrates the potential of a chemometrics-assisted approach to quantitative handheld LIBS analysis.

Using 17 silica-based reference materials and a combination of spectral preprocessing, Kennard–Stone sample selection, PLS regression, and VIP variable selection, the researchers developed and validated quantitative models for 19 elements using a **SciAps Z-903.**

The resulting calibration was then applied to archaeological materials in the field, demonstrating how quantitative elemental information can contribute to the investigation of artifacts **without requiring every sample to be transported to a laboratory**.

The study also highlights an important limitation: a calibration developed from a particular material class is not automatically applicable to every material. The researchers note that the relatively narrow diversity of their silica-based standards limits the scope of the calibration, and that additional optimization is needed for rough or heterogeneous artifact surfaces.

For researchers developing their own LIBS applications, the broader lesson is clear: **quantitative handheld LIBS begins with a well-designed calibration**.

With appropriate standards, measurement protocols, preprocessing, modeling, and validation, broadband LIBS spectroscopy can move beyond rapid elemental identification to provide meaningful quantitative information—even in applications where laboratory analysis is difficult or impractical.

Original Research:

Lando, G. et al. “Chemometrics-Assisted Calibration of a Handheld LIBS Device for the Quantitative Determination of Major and Minor Elements in Artifacts from the Archaeological Park of Tindari (Italy).” Applied Sciences, 2025, 15(12), 6929. DOI: 10.3390/app15126929.

Read the original study