

Supplementary information

Improved mineralogical analysis in copper ores by Laser-induced breakdown spectroscopy

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Table S1. Number of samples in the sets of calibration (Cal), validation (Val) and testing, according to the chemometric models applied.

| Mineral | Final Models Samples | PLS (Cal/Val) | ANN (Cal/Val/Test) | MCR-ALS (Cal/Val) |
|---------------------|---------------------------------|--------------------------|-------------------------------|------------------------------|
| Bornite | 80 | 56 \ 24 | 56 \ 16 \ 8 | 56 \ 24 |
| Chalcopyrite | 78 | 55 \ 23 | 55 \ 16 \ 7 | 55 \ 23 |
| Covellite | 81 | 57 \ 24 | 57 \ 16 \ 8 | 57 \ 24 |
| Enargite | 81 | 57 \ 24 | 57 \ 16 \ 8 | 57 \ 24 |
| Iron Oxides | 76 | 54 \ 22 | 54 \ 15 \ 7 | 54 \ 22 |
| Molybdenite | 74 | 52 \ 22 | 52 \ 15 \ 7 | 52 \ 22 |
| Pyrite | 80 | 56 \ 24 | 56 \ 16 \ 8 | 56 \ 24 |
| Quartz | 81 | 57 \ 24 | 57 \ 16 \ 8 | 57 \ 24 |

Table S2. Additional parameters for MCR-ALS with correlation constrains in mineral species calibration.

| Mineral | Convergence criterion | Std. Des. Residuals | LOF (% Exp) | LOF (% PCA) | r² |
|---------------------|----------------------------------|--------------------------------|------------------------|------------------------|----------------------|
| Bornite | 0.1 | 0.110 | 1.192 | 1.093 | 99.99 |
| Chalcopyrite | 0.2 | 0.008 | 0.840 | 0.729 | 99.99 |
| Covellite | 0.1 | 0.007 | 0.668 | 0.627 | 99.99 |
| Enargite | 0.1 | 0.016 | 1.713 | 1.534 | 99.97 |
| Iron Oxides | 0.1 | 0.008 | 0.776 | 0.613 | 99.99 |
| Molybdenite | 0.1 | 0.003 | 0.350 | 0.281 | 99.99 |
| Pyrite | 0.1 | 0.008 | 0.790 | 0.731 | 99.99 |
| Quartz | 0.1 | 0.072 | 5.608 | 3.947 | 99.68 |

Figure S1. Elemental data conciliation of copper (Cu), iron (Fe) and sulfur (S) with SEM-MLA.

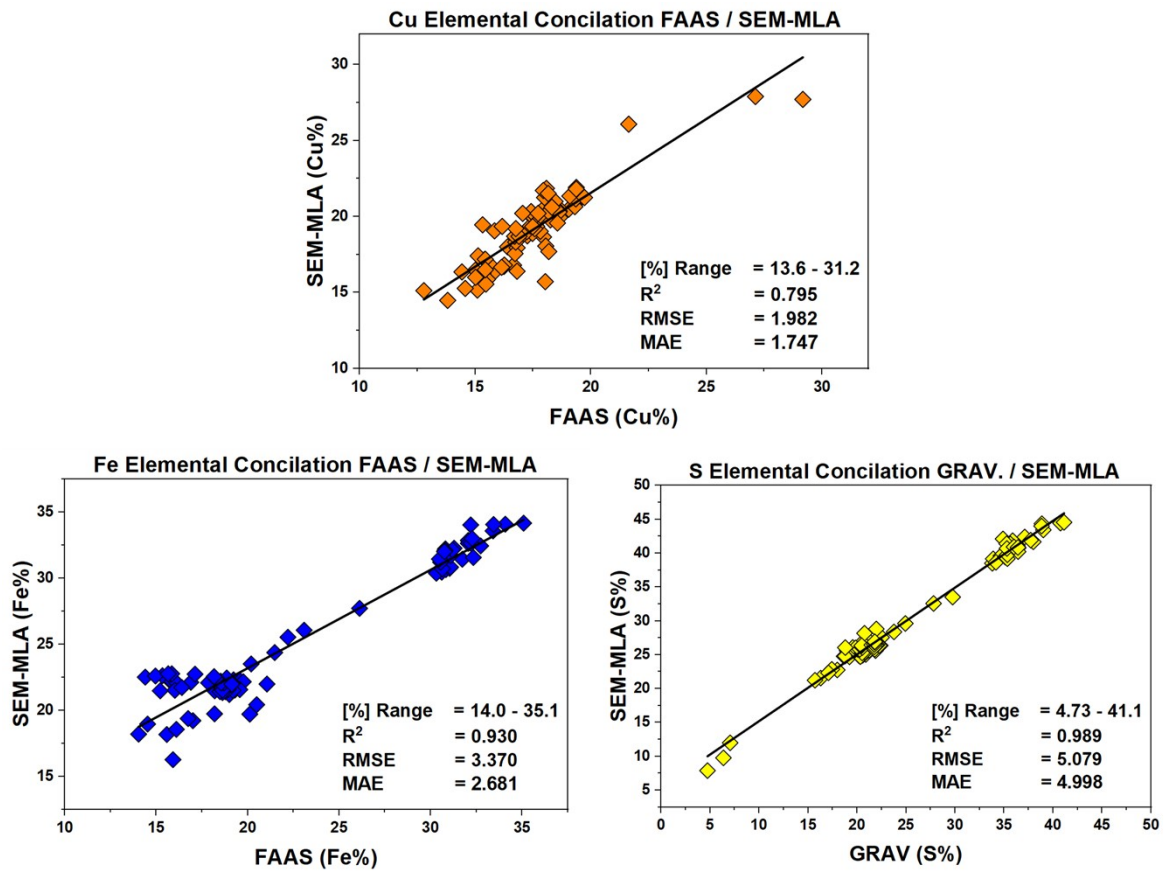


Figure S2. Regression vectors achieved in PLS models for mineral species in copper concentrates.

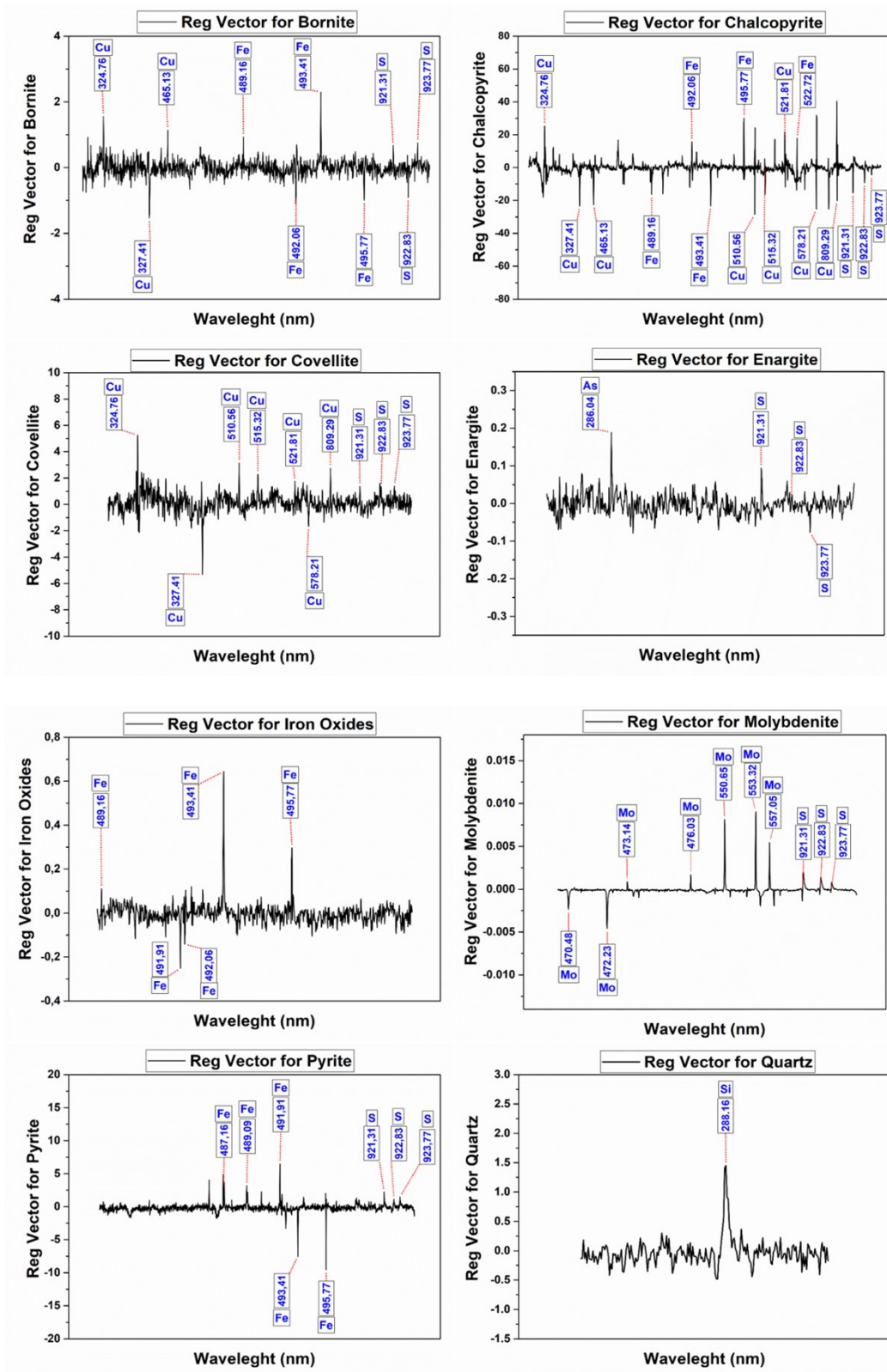


Figure S3. MCR component vs reference spectra (spectral profile) and total spectra reconstructed (CS^T) by MCR-ALS with correlation constrains for the mineral species.

