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Multivariate classification and quantification of sedimentary rocks analysed using stand-off Laser-Induced Breakdown Spectroscopy system

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In this study we present a robust Laser-Induced Breakdown Spectroscopy (LIBS) device capable of stand-off (from 6 to 20 meters) as well as remote sensing, the so called X-Trace specially designed by AtomTrace (CZ). All the samples were measured at the distance of 9 meters in collinear arrangement; axes of the laser beam and the collecting optics were identical. The plane of the sample surface was placed perpendicular to the analytical axis of the stand-off system, allowing the best conditions for LIBS analyses. Samples of 28 sedimentary rocks distributed in four different rock matrices were analysed in the form of pressed pellets. Afterwards, the obtained data set was treated with multivariate algorithms. For classification, linear algorithms based on least squares method (soft independent modelling of class analogies (SIMCA) and partial least squares discriminant analysis (PLS-DA)) were utilized and their performance was compared to that of artificial neural network algorithm. In the case of quantification, results obtained using principal component regression (PCR) and partial least square regression (PLSR) were compared.

[1] El Haddad J et al. (2014) Spectrochimica Acta Part B: Atomic Spectroscopy 101: 171-182. DOI: 10.1016/j.sab.2014.08.039.

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