

A unique AI/ML based approach for the semiquantitative analysis and calibration-free multielement screening of different terrestrial materials using ICP-OES

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Geological studies often require the precise determination of isotopic composition and isotopic ratios of elements in a variety of different terrestrial materials including rock, soil, and water samples. Some applications include Sr isotopes for provenance studies, U-Pb dating for chronological investigations, development of new reference materials etc. A multi collector inductively coupled plasma mass spectrometry (MC-ICP-MS) is commonly used to detect the minimal isotopic variations in such samples with sufficient precision. Whilst the technique excels with highest sensitivity and unmatched precision, sample cleanup and characterization are required since even trace amounts of contamination coming from the sample matrix, diluents and/or analytical systems could lead to inaccuracies in the results.

Prior to analysis with MC-ICP-MS, the prepared solutions are commonly screened using a robust and quantitative technique such as inductively coupled plasma optical emission spectroscopy (ICP-OES). Modern ICP-OES systems offer low detection limits and can detect multiple elements in a single exposure, but require calibration for quantitative information, which can be time-consuming and limit element screening. For completely unknown samples, analytical re-runs may be necessary to ensure quantification using calibration standards in correct concentration ranges for the different elements. An innovative AI/ML-based semiquantitative approach can expedite this process, providing multielement data without calibration standards and save significant time and effort.

This study compares the fully quantitative and semiquantitative analyses of geological and environmental samples, such as leachates and rock digests of unknown samples as well as reference materials, using ICP-OES to illustrate the usability of the technique in various geological applications.