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Automated sample identification with SpectPro and PTAL database for the analysis of spectra from planetary missions

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The Planetary Terrestrial Analog Library (PTAL) is a database in which spectroscopy scientists have gathered spectroscopic data with Raman, LIBS, NIR and XRD techniques, of samples relevant for the analysis and data exploitation of planetary missions such as ExoMars. The SpectPro tool is an application developed in the framework of the development of the RLS Raman instrument of the ExoMars mission that provides an analytical set of tools capable of analysing the scientific and housekeeping data received from the RLS instrument (this section of the software is referred to as IDAT), but also from other sources, with a set of available functions for the comprehensive analysis of spectroscopic data, including operations such as binning of images, baseline removal, filtering, SNR calculation, normalization, a spectra calculator, automated peak detection... The SpectPro and PTAL teams have worked together to facilitate a direct access from SpectPro to the PTAL database, using the same credentials for access to the PTAL web interface. This connection will boost the capability of the scientist working in a planetary mission (but not only) to perform a fast and comprehensive characterization and identification of the mineral phases present in a sample by comparing the data obtained from the sample with the extensive spectral information included in the PTAL database. This will be possible by profiting from the navigation pane included in SpectPro. In addition, using the peak detection capabilities of SpectPro, it will be possible to perform sample identification based on the acquired spectra. In this work the results of the merging effort between PTAL and SpectPro will be presented, with focus on the analytical capabilities of the software, especially the automated peak detection methods and sample identification routines implemented, which allow the identification of compounds by taking into account the peak information stored in the database, and crossing it with the automatically detected peaks on the processed spectra. These methods make use of all the peaks of the spectrum, providing accurate results also for admixtures.

Reference

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