

DATA PROCESSING SOFTWARE FOR LA-ICP-MS

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The modern use of LA-ICP-MS often require hours of work after data acquisition, especially as the elemental imaging is becoming more desired. Relatively few non-commercial software tools are available to assist with this process.

The goal of this work was to create free, open source desktop application for fast processing and visualisation of mass spectrometric data. Our intention was to create simple, easy to use interface that will offer the first look on acquired data with no need of any preparation. This program was created using programming language python¹ and the user interface was built on top of the standard library tkinter. Using PyInstaller² program we created a one file executable, that can be used under Windows without the necessity of installing python or any other packages.

The program is aimed on data created with laser ablation inductively coupled plasma mass spectrometry. It is suited for a spot and line analysis as well as an elemental imaging. The data can be imported directly from mass spectrometry data acquisition as .csv files. The program presents two ways of data evaluation; either calculating the mean of the peak values or using a peak integration. The automatic selection of the background and sample intervals from time resolved data is shown in the main window. There is an option to check every element in an interactive graph with highlighted background versus sample time view. This program also allows user to choose from 2 possible correction procedures; correction on internal standard and sum of oxides correction. Using a certified reference values, it calculates the content of measured elements. It is possible to export data at any step of the evaluation; data are exported into an excel sheet. It is also possible to create calibration curves. The intercept and the slope calculated in calibration window can be directly used for the creation of elemental maps.

1. Rossum, Guido van, et al, 'The Python Language Reference', Python Software Foundation;
<http://docs.python.org/py3k/reference/index.html>
2. <http://www.pyinstaller.org>