

Nu Instruments Calculations Editor (NICE) Customized Charts for Reporting in Nu Quant

- Graphical data in user defined format
- Customized labelling with dynamic values
- Scatter, line and bar chart types mixed as required
- Edit sample input parameters from the charts

The Nu Instruments Calculations Editor (NICE) is a powerful tool that allows users to process numerical data in the way they want. Using NICE allows the calculation of results to be scripted and used over multiple samples easily and quickly. Scripts generated in one batch of samples are saved for global use in other batches and can even be exported for transfer to other computers when required.

As scripts can be simply imported and exported, there is a library of scripts available to either be used directly or easily modified for the specific isotopes being measured and data that needs to be reported. The following are examples of some of the charts that have been generated using NICE for different applications. Assistance to customize NICE scripts for new applications is available through the Nu Instruments Applications team.

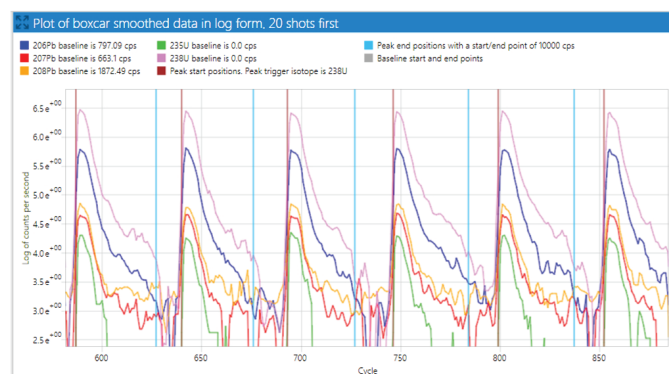
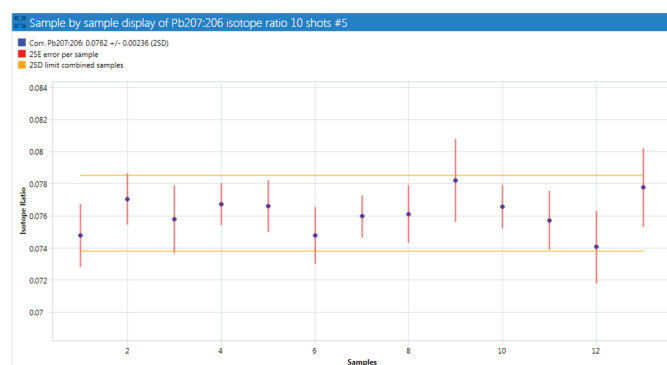
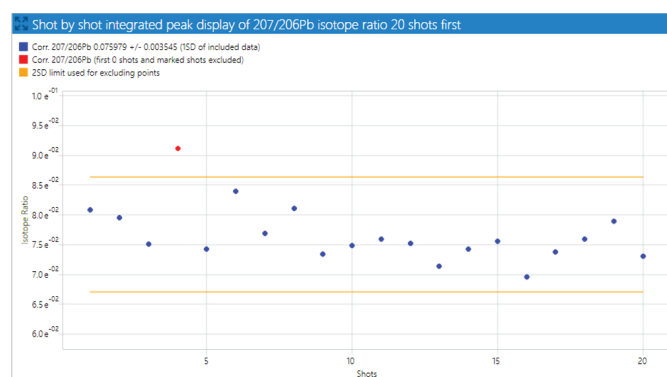
Applications of charts in NICE

The NICE charts can show overlaid data to allow visualization of signals, this example shows single shot laser ablation of the zircon standard 91500 using a fast washout cell.

When the scripts are used to process the data within certain boundaries, the chart is used to display the boundaries and

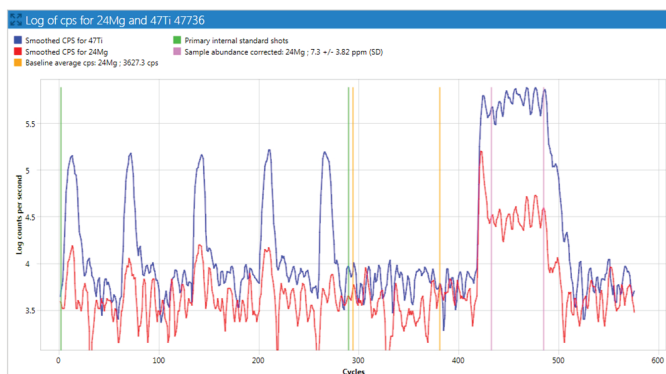
When a series of samples of the same type have been measured, a chart can also display the mean of each sample with individual error bars and statistical boundaries for the sample group.

A script can also allow regions of interest to be defined manually as in this example of a specialized laser ablation method for Sapphire. Single shots of smaller spot size are used to determine the internal standard ratio of a secondary internal standard (^{47}Ti) against the primary internal standard (^{27}Al) which would be too intense to measure accurately with the larger spot size needed to detect the trace elements such as ^{24}Mg .

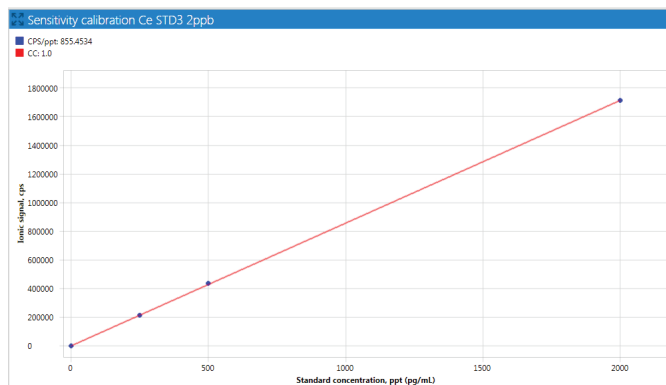


allow editing for recalculation. The example above shows the markers from an automated search for peaks with user pre-defined parameters. These parameters are variable for each sample in the sample list or directly from the chart.

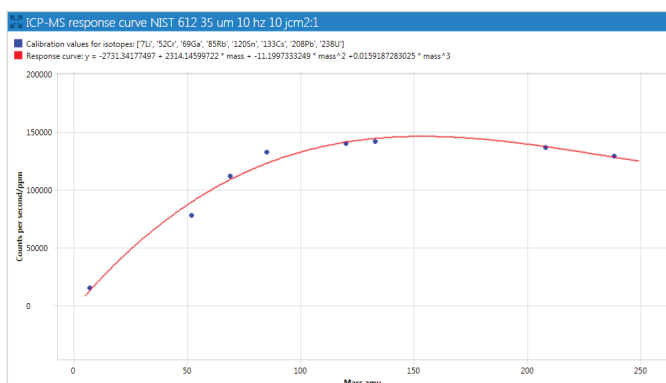
For conventional isotope ratios, the NICE chart will display the individual measured ratios for each cycle and display the included and excluded ratios used to calculate the mean for the sample. The statistical boundaries of the measurement are displayed and the chart labels will display the mean and standard deviation of the cycles (which are also displayed in the tabulated data).



The charts are also used to display the calibration information from a NICE script, in this example a calibration has been derived from ionic standards used to calibrate the sensitivity for a nanoparticle data set.

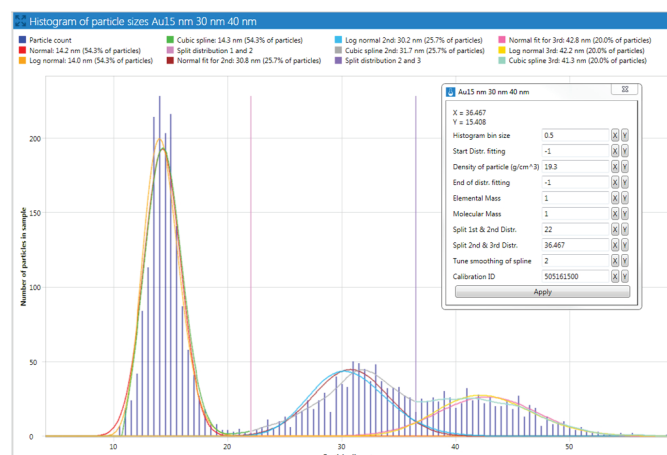
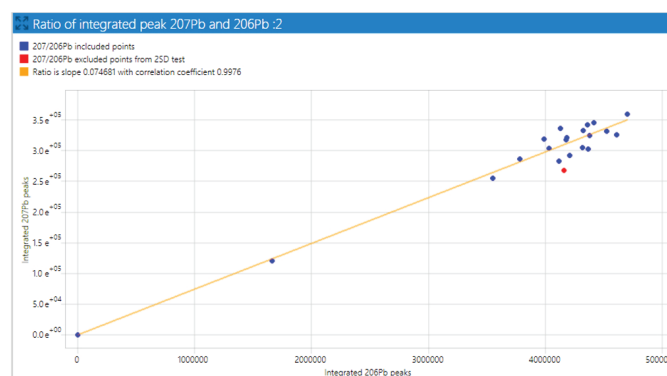


The NICE script will also calculate curve fits which can be displayed in the chart. In this example a 3rd order curve has been fitted to the sensitivity data for a range of isotopes. This is then used to generate a mass response curve so laser ablation sample concentrations can be calculated.



The charts can also be used to visualize more specialized techniques such as the calculation of an isotope ratio from the integrated area counts from a range of laser ablation spots. In this example, the raw data of one isotope's signal is plotted against a second isotope. The slope of the linear regression, forced through the origin, is the required ratio (the excluded points are based on a 2 Σ exclusion of the individually calculated ratios).

The charts can represent complex data with mixtures of scatter, line and bar chart display types with flexible labelling to include calculated values. The input variables for the sample can also be accessed from the chart using the mouse cursor position as a data point for entry if required. In this example, the histogram for a mixed size nanoparticle sample is displayed along with the normal, log-normal and cubic spline fitting of three different regions representing the three particle distributions.



Conclusion

The Nu Instruments Calculations Editor (NICE) allows data processing scripts to be used as exchangeable templates between batches of samples and even between laboratories. The implementation of charting into the NICE scripts in Nu Quant allows for flexible customized charts to be used to display the data in the best way for the methodology adopted by the user.