

Nu Instruments Calculations Editor (NICE) for Nu Quant

- Simple copy and paste to apply a NICE script to multiple samples
- Recall function to use values from one sample to another
- Simple methods to apply variable changes to a whole batch of samples
- Methods for internal and external mass bias as well as isotope dilution techniques

AttoM can be used to analyse samples for quantitative measurements and highly precise isotope ratios. The processing of data for isotope ratios requires a variety of calculations depending on the type of correction needed and the analyst's choice of calibration technique. Nu Instruments has always provided users with a flexible method of implementing customized calculation routines with a proprietary Nu

Instruments Calculations Editor, NICE. NICE has now been augmented for use with Nu Quant and changes made to implement a standard programming language and syntax (Python) as well as simplifying the ability to use NICE with batches of samples rather than a sample by sample implementation.

Nu Quant NICE uses the simplified dashboard display with the ability to show the details of each summary reported value. This includes the calculations for each individual cycle along with which cycles are excluded from the user settable rejection test. Nu Quant also preserves a change history showing what was changed for each sample, the previous value, when it was changed and by whom.

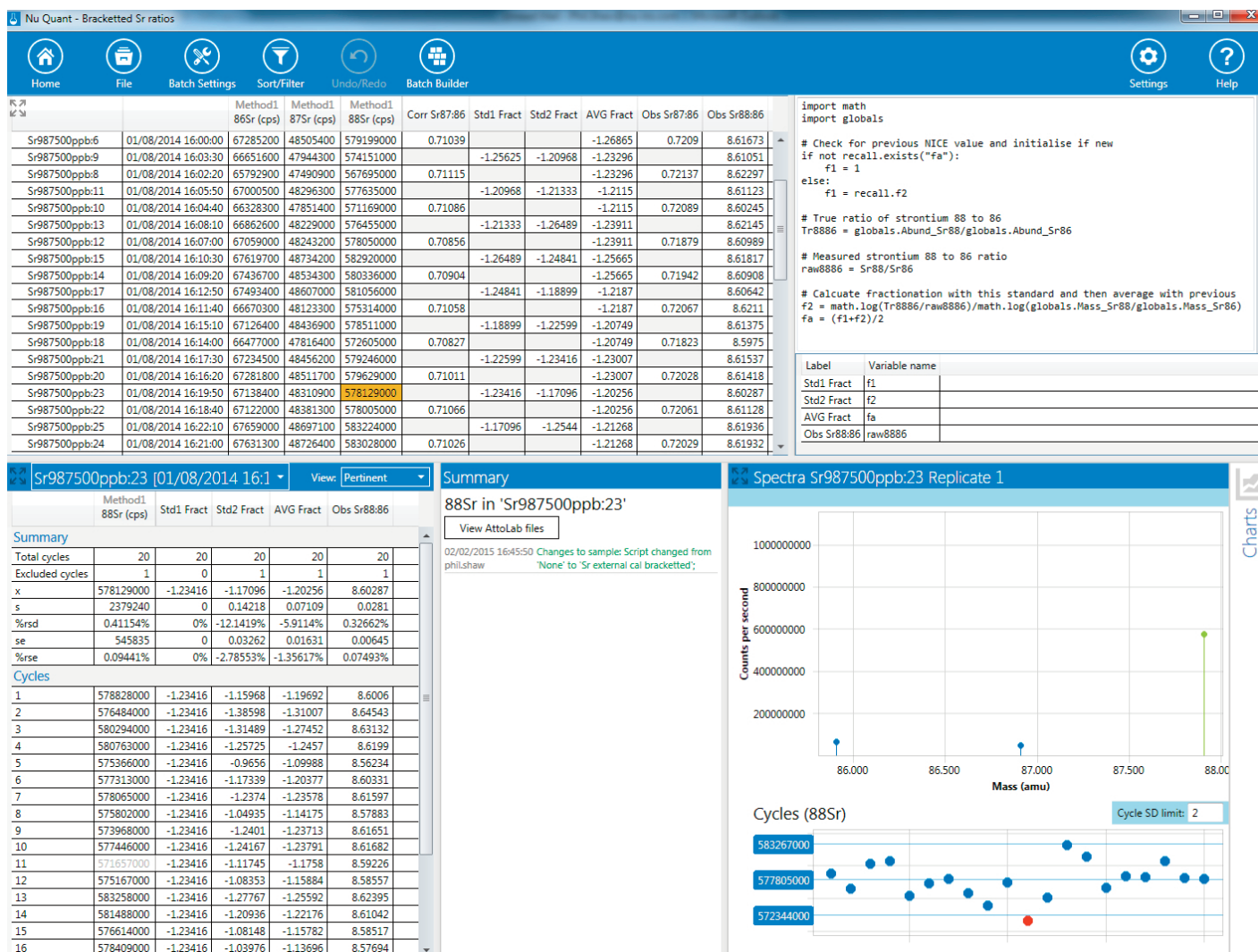


Figure 1: An example display of a batch of samples using an isotope ratio method with sample/standard bracketing to calculate mass bias

The script editing tools provide an intelligent code check system so each variable can automatically be recognized as correct and variables can also be selected by double clicking on labels in four simple library lists shown next to the editor:

- **Input variables** – which may change from sample to sample and can be modified for each sample by copy of paste in the sample list.
 - The concentration for an Isotope Dilution spike
- **Output variables** – calculated using the NICE scripts and reported for each cycle and sample.
 - An isotope ratio
 - A mass fractionation factor

- **Application variables**
 - The cycle ICPS for an isotope
 - The mean ICPS for an isotope after the SD exclusions for that sample
 - The standard deviation of the ICPS for an isotope after the SD exclusions for that sample
 - The number of cycles included in the mean and SD for each isotope
 - The total number of cycles measured in the method
- **Global variables** – user editable constants that do not vary and can be defined for use across multiple batches.
 - The masses of isotopes
 - The natural abundances of isotopes
 - Reference material values

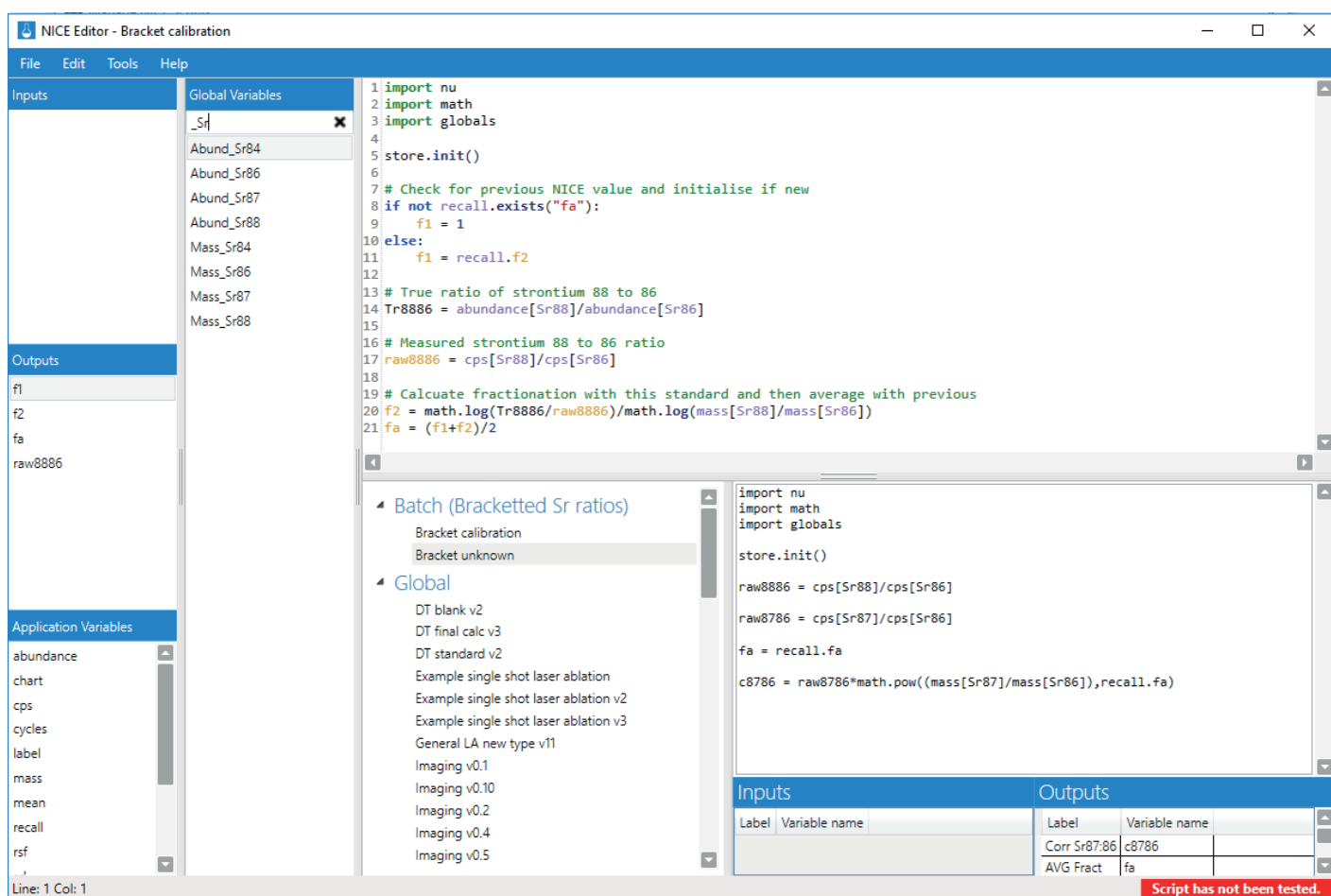


Figure 2: The NICE script editor with intelligent code checking and simplified variable libraries as well as a built in browser to compare and copy from other scripts