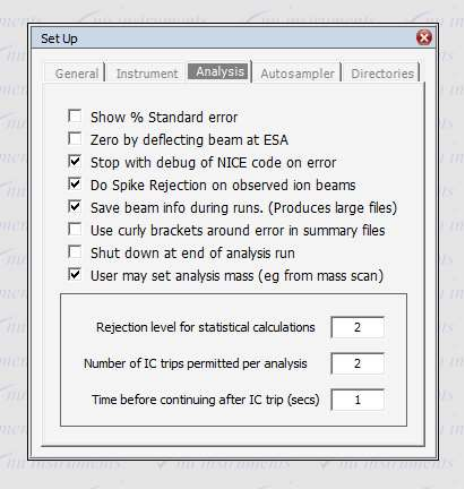
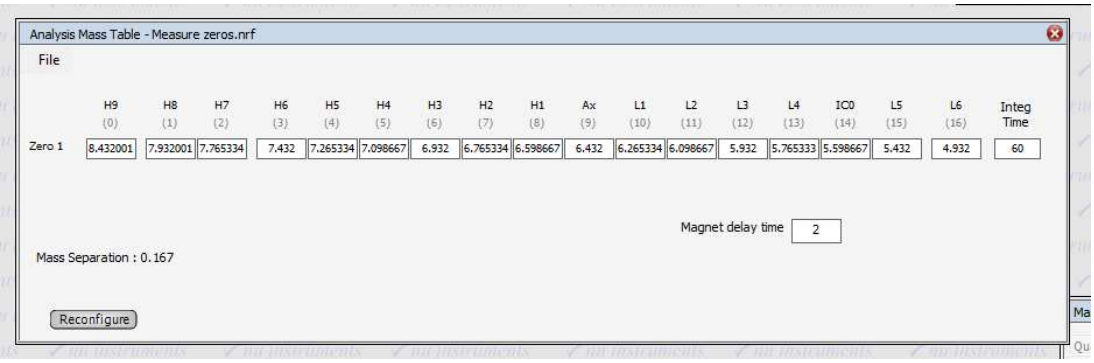
Peak centring notes for NuPlasma3, April 2021

A. To run without peak centring (i.e. usual method to use for Li isotopes)

A1. Go to ***Setup – Preferences – Analysis*** and ensure ***User may set analysis mass (e.g. from mass scan)*** is ticked. *(This will allow you to manually set the magnet mass before the run and leave it fixed at that value for all measurements during a batch run)*

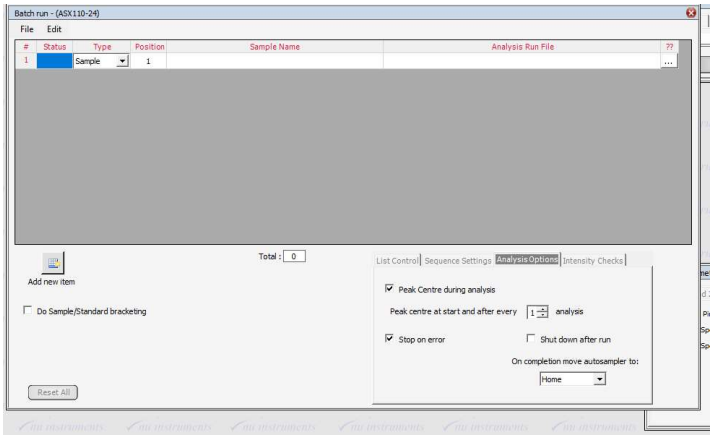


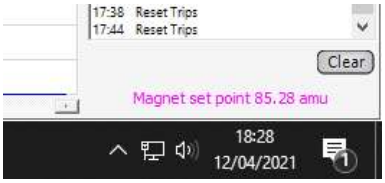
A2. Open ***Data Acquisition – Analyse – Old Routine – Measure zeros***, and just check that the centre mass position in the mass table corresponds to the element and configuration you are measuring (e.g. around 6.43 for Li). This does not have to be perfect – within ~0.1-0.2 should be ok. *(N.B. There should be no need to change this nrf file as we have set up separate 'Measure zeros' files for Li and Sr, and we can do the same for any other elements if we wish. For Li, it is called 'Measure zeros'; for Sr, it is 'Measure zeros_Sr'. But if it does ever need to be changed, you need to (i) click on reconfigure and type in the appropriate mass separation (if switching to a different element), (ii) return to the mass table, double-click on the Axial box, type the correct mass number, and hit return for the other positions to fill in manually, and (iii) go to 'File – Save as' and re-save with the same file name.)*



A3. After tuning and before starting a batch run containing samples, you should run standard stability checks as usual with peak centring switched on (one measurement would be enough for the purpose of peak centring, but you'll presumably measure more than this if running a stability check!). Note down the peak centre position while it is measuring a standard – this can be observed

during measurement in the bottom-right of the screen (labelled ***Magnet set point: XXX amu***), but it is probably best to check this in a Results file for a standard from this run i.e. where it says ***Axial Masses used: XXX*** *(N.B. NOT where the Result file says 'Zeros measured at centre mass XXX' – this could be a magnet mass from a blank in a previous session which might well not be appropriate).*





NBS987 (Results #13544) - Notepad

File Edit Format View Help

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Sample name : NBS987
Run File    : C:\Nu Plasma Files\Analyses\Sr H6.nrf
Operator    : Philip

Tau Correction invoked
Raw data is stored in file: C:\Nu Plasma Files\Results\2021-4-12\NBS987 (Data #13544).t

Zeros used obtained on :  Apr 12 2021 at :  15:54
Zeros measured at centre mass   85.25

Background signal (3) = 2.875882E-03
Background signal (5) = -3.965871E-03
Background signal (7) = -1.990797E-03
Background signal (9) = -4.291352E-03
Background signal (11) = -4.966991E-03


           Axial Masses used : 85.254

Block Number: 1                        Mean         StdErr   Num Measurements

        87/86 bias corr            7.101461E-01    1.53E-05     9 out of 10
        87/86 bias + Rb corr       7.101483E-01    1.55E-05     9 out of 10
        84/86 bias corr            5.655091E-02    6.98E-06    10 out of 10
        86/88                      1.150874E-01    1.93E-06    10 out of 10
        Fract                     -1.601385E+00    7.31E-04    10 out of 10
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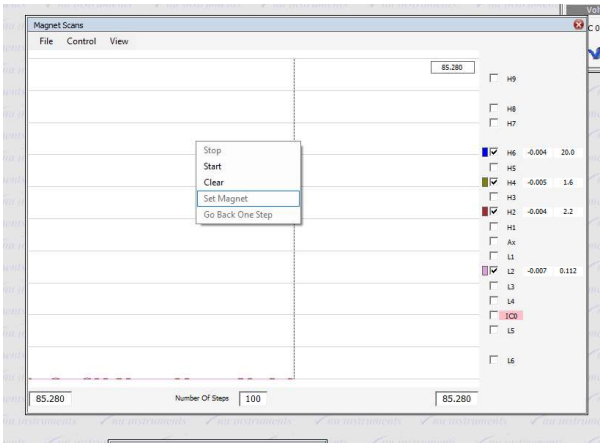
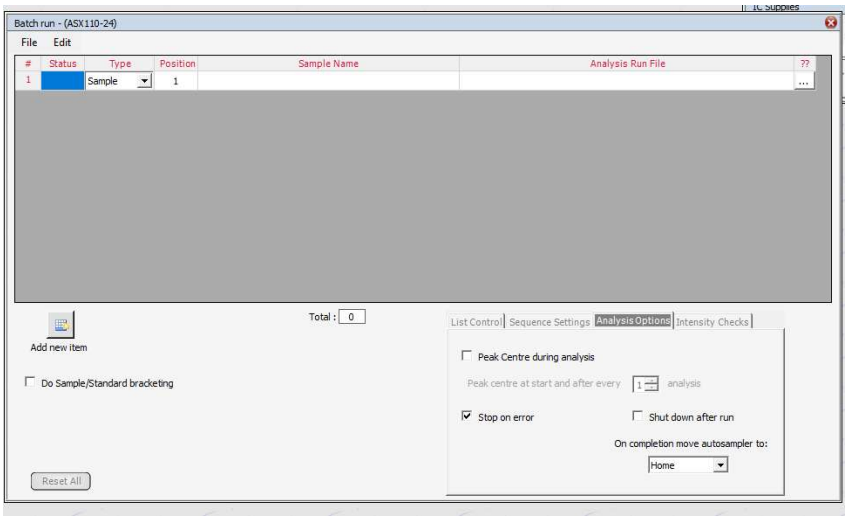
A4. Go to ***Scan – Magnet*** and then manually set the magnet at this exact mass position *(This is very important – as all the analyses will all be conducted at this magnet position.)*



A5. For the batch run, make sure ***Peak Centre during Analysis*** is NOT ticked, so that it does not attempt to peak centre, and it will therefore use this manually set mass position for all standards/samples and blanks throughout the run. *(If you did run with peak centring ticked here, it will peak centre on samples, but revert to the manually set magnet mass for blanks. This allows for drift only for samples but not for blanks, although in practice this should also be ok…)*



B. To run with peak centring (N.B. this is 'exploratory'; not our usual method for Li)

In theory, it should be possible to use the peak centring from samples/stds within a run to set the magnet position for intervening blank measurements. The instructions from Nu didn't seem to work properly and we're still looking into this… But the following did seem to work for me for Sr. A word of caution here: I've not tested this for other elements and so it's probably worth checking it behaves like I've described here the first time you try for yourself, particularly for a different element. Note that all steps B1-B5 are in some way different from A1-A5 above!

B1. Go to ***Setup – Preferences – Analysis*** and ensure ***User may set analysis mass (e.g. from mass scan)*** is NOT ticked.

B2. Open ***Data Acquisition – Analyse – Old Routine – Measure zeros***, and check that the centre mass position in that nrf file (e.g. 'Measure zeros.nrf', or 'Measure zeros_Sr.nrf') corresponds EXACTLY to the centre mass position in the nrf file for the isotope analysis (e.g. 'Li Philip2.nrf'). *(This is important in order for the peak centring from standards to lead to it measuring the blank in the same position. If it needs to be changed, see instructions in A2 above.)*

B3. Before starting a batch run containing samples, you should run standard stability checks as usual with peak centring switched on *(This is because it's necessary to make sure the instrument measures a peak centre on at least one standard/sample before it tries to measure a blank in your batch run. Alternatively, start a batch run with a standard as a 'dummy').*

B4. Strictly it might not be necessary to go to ***Scan – Magnet*** and manually set the magnet, as the std/sample nrf file tells it which mass to go to when it first peak centres. But I didn't have a chance to test this, and I'd say you might be best off still doing this anyway!

B5. For the batch run, make sure ***Peak Centre during Analysis*** is ticked. It will peak centre on each standard/sample and then use the most recent peak centre settings for the intervening blanks. *(N.B. It looks like this method should allow the 'magnet drift' from samples to be applied to blanks as well. But it only works properly if the centre mass for the two nrf files is set to be exactly the same; if they are set slightly differently it will offset the mass it measures blanks at according to that difference, and we don't want it to do that!)*