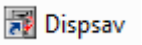
Using Proteus and Dispsav to Process Evolved Gas Data (8/12/15 edits highlighted)

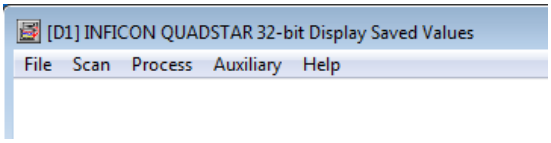
Once MS data has been acquired for the gases evolved during your DSC/TGA run, you will process using Proteus software. You may also find Dispsav, part of the Aeolos software suite, to be useful, *but probably not.* SKIP TO PAGE 5 FOR PROTEUS!

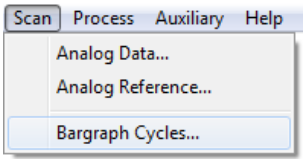
Using Dispsav to Process the Data (included but not recommended)

Open the Aeolos_III suite of programs 

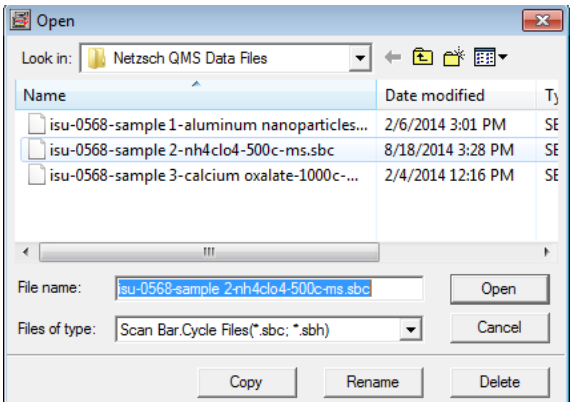
. Select Dispsav 

. A rather sparse pull-down menu will initially be displayed:

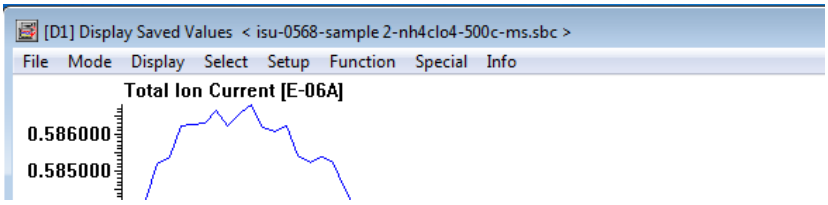


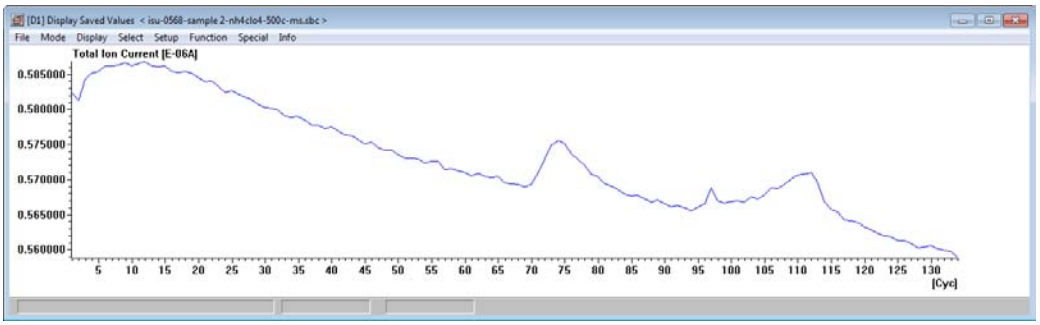


Select Scan -> Bargraph Cycles . Navigate to the file of interest. Select and Open.

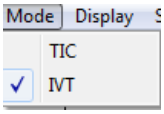


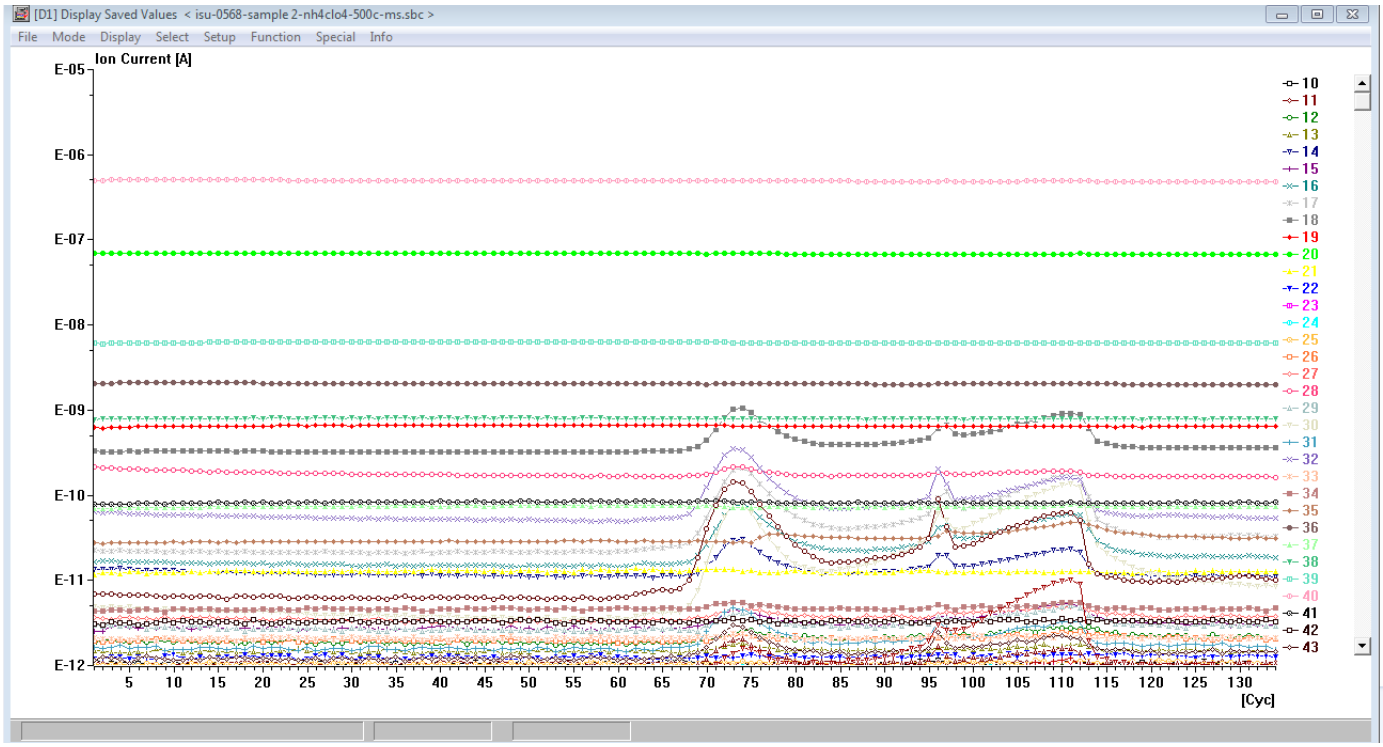
The view may initially show the TIC (total ion current vs cycle number or time) and will have more compete pull-down menus.





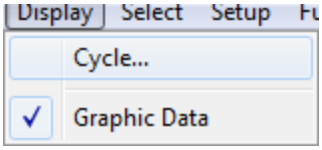
Change the display Mode from TIC to IVT (ion values vs time).

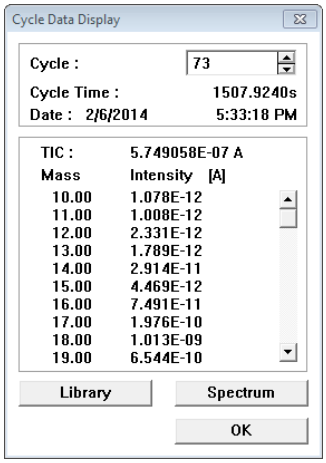


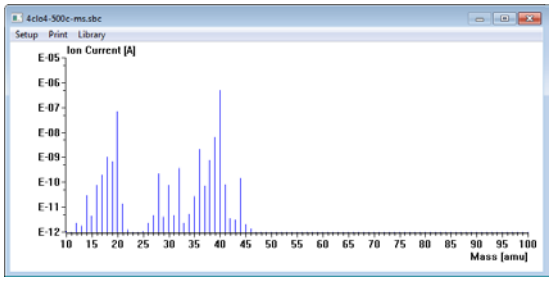


Note that there are unique symbol/color designations for each mass in the scan, and that the y-axis is typically a log display. Take note of the cycles that appear to have the most useful data. In this example we will focus on the first major peak, typified by cycle 73; a reasonable baseline for subtraction might be cycle 60.

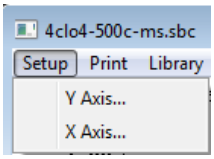
Select Display -> Cycle. A dialog box will appear allowing you to view a list of the masses in each cycle. Choose cycle 73, and select Spectrum.



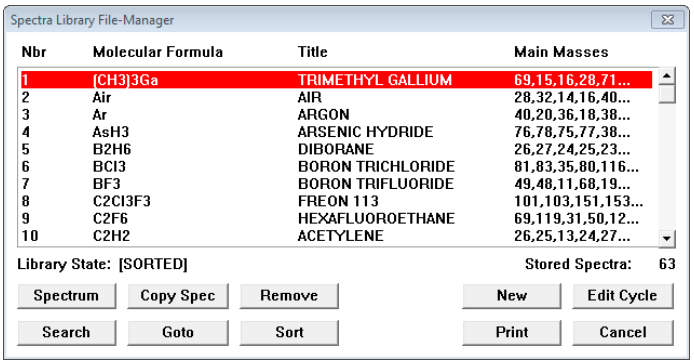




Note that you can change the nature of the y-axis display between linear and logarithmic, but there is no convenient way to autoscale.

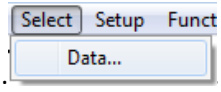


Selecting “Library” from either the Cycle Data Display or the Spectrum display will open a text view.

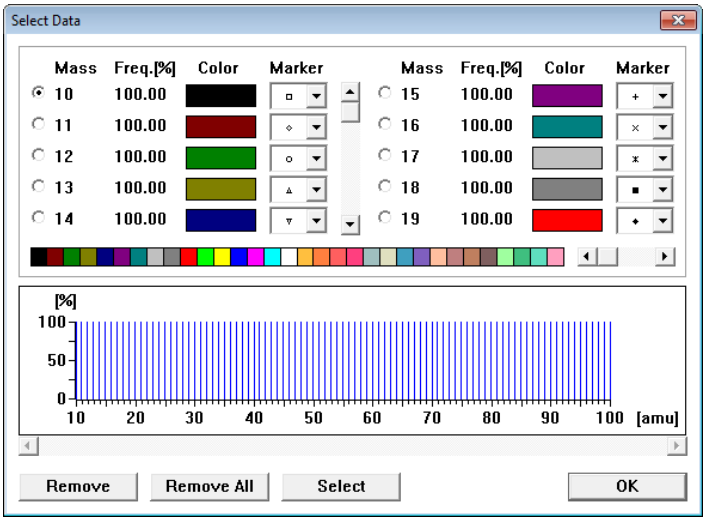


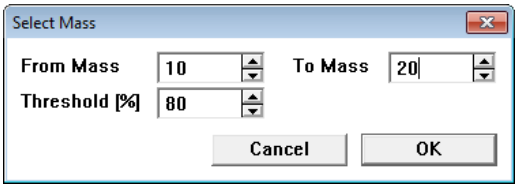
Be aware that some of the button choices are known to crash the program. It may be useful to incorporate this program into the workflow once we understand it better, but no additional program help will be given at this time.

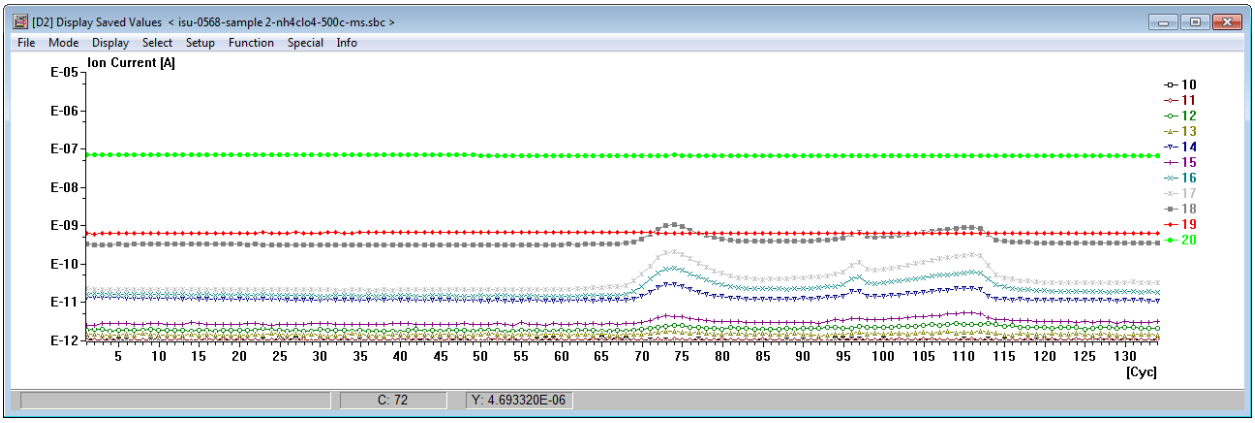
Return to the main Dispsav view. The multi-curve display of masses vs cycle number should be present. It can be helpful to go through the mass traces in more detail in order to find all of the cycles with useful information.

Choose Select -> Data… 

Then choose Remove All, followed by Select. This will open a dialog box to allow you to choose a narrower range of masses to view. For example, try working through the mass range 10 values at a time, taking note of important cycles.



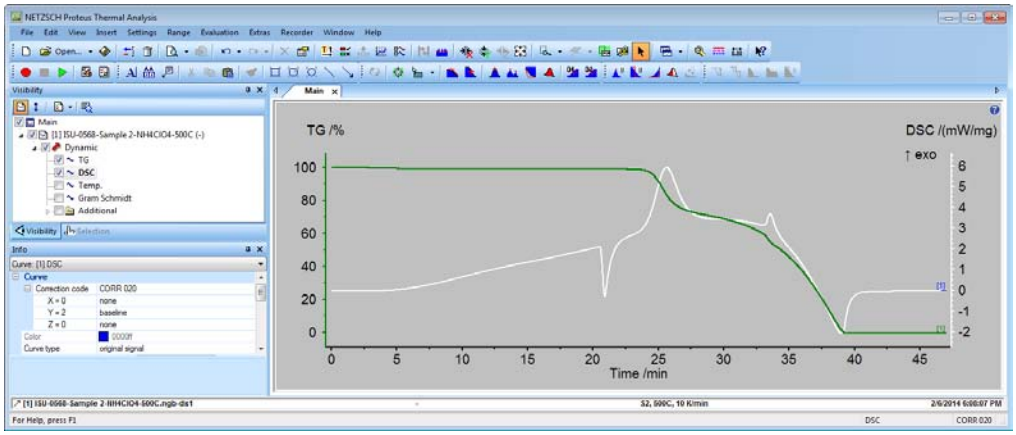




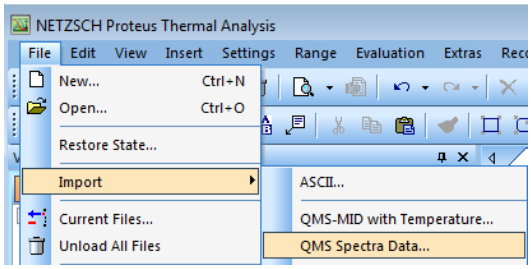
That's about all Dispsav can be used for at this time.

Using Proteus to Process the MS Data

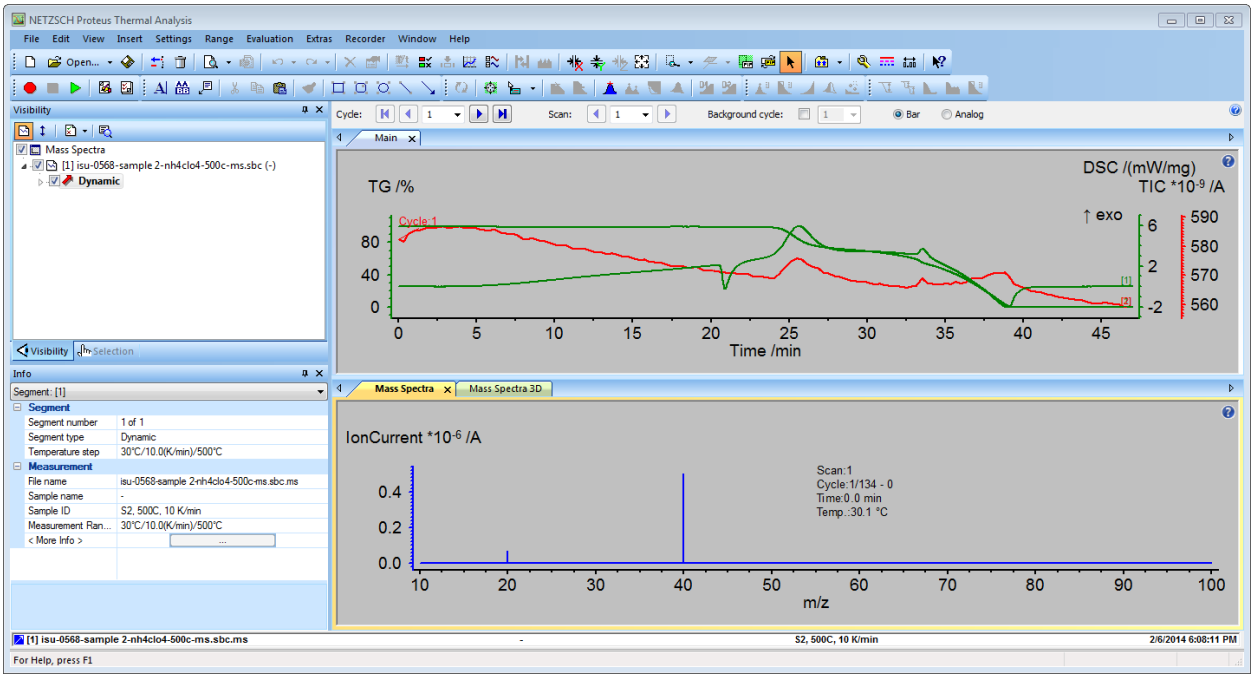
Start Proteus. Open the DSC/TGA data file that was acquired with the MS data. Select only the TG and DSC signals for viewing. Select one of the traces in the view.



From the File pull-down, choose *Import -> QMS Spectra Data*.

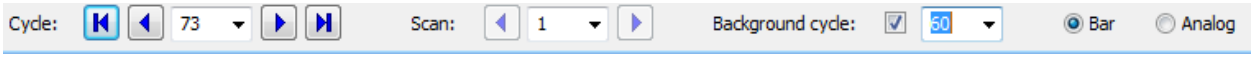


Navigate to the QMS data file that corresponds to the TGA/DSC acquisition. Select and open it. The Proteus view should now look like:

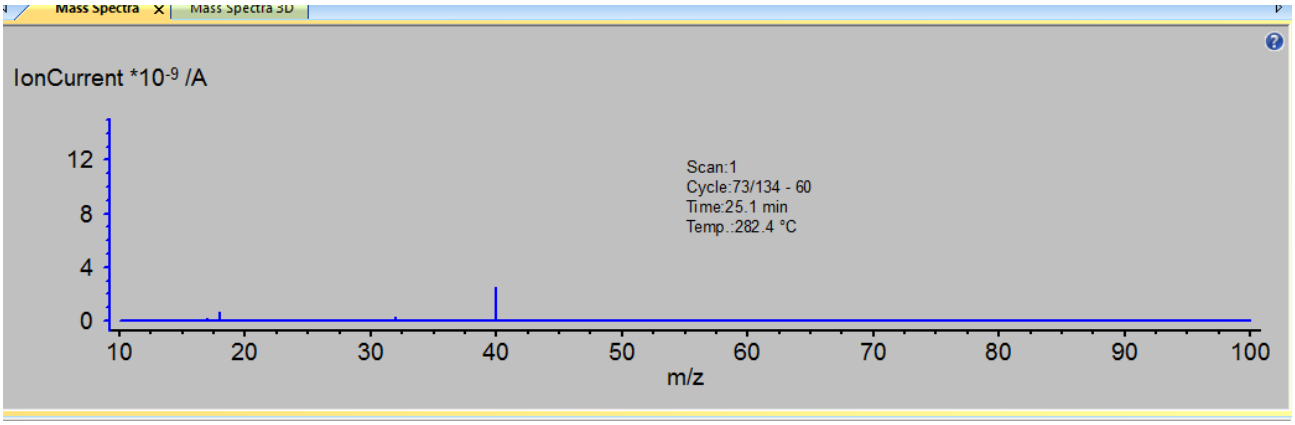


The upper view with just one tab will show the TGA/DSC curves and the TIC (total ion current) trace. The lower view with two tabs will show the mass spectrum of the cycle selected (defaults to cycle #1) and the 3-D view of spectra versus temperature. (The 3-D view is fun to play with, but it's not clear how valuable it is as part of normal data processing.)

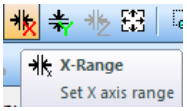
The Cycle ribbon bar is now visible:



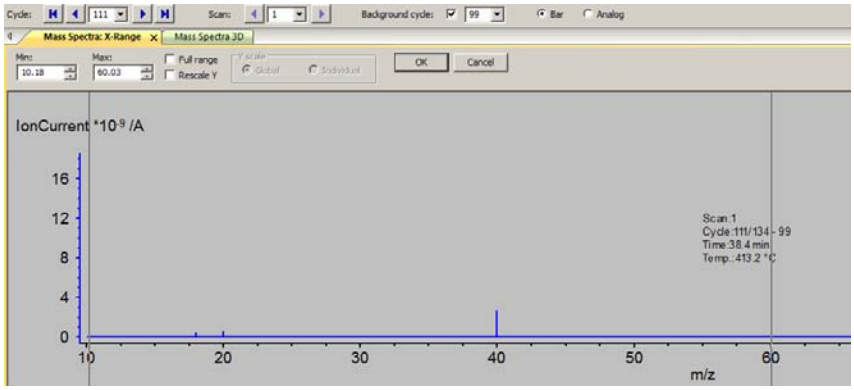
For "scan bargraph" data, "scan" will always be set to 1. On the Cycle bar, select cycle 73 to view, and cycle 60 to be subtracted as the background. You may see something like this:



To rescale the spectral display, set the x-axis first!

Use the "X-range" tool on the ribbon bar 

to adjust the m/z axis to show from 10 to 60 Daltons. Click and drag the vertical lines, then select OK to apply to the view.



Next, use the "Y-range" tool 

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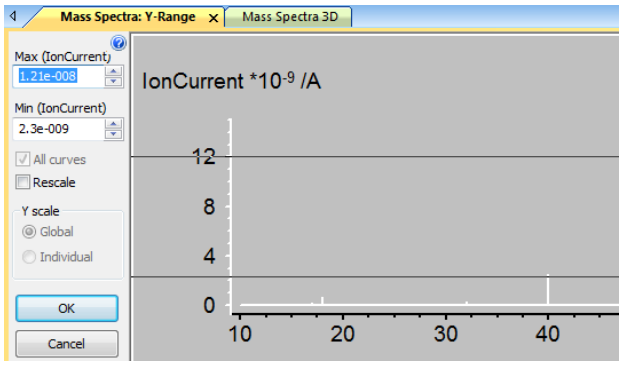
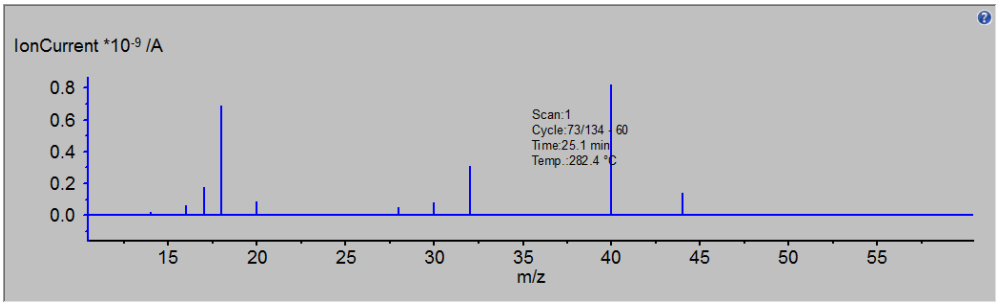
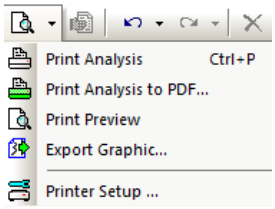


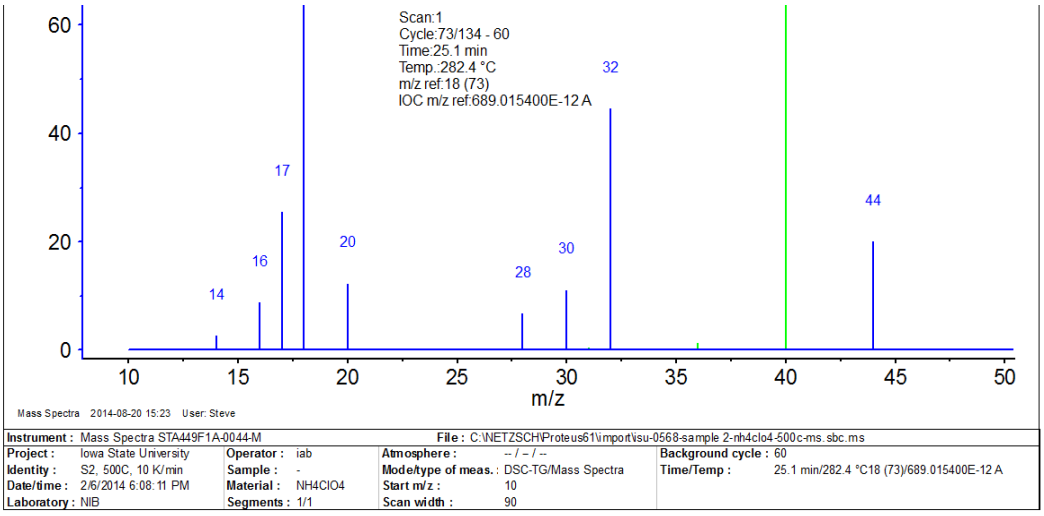
Click and drag the two horizontal black lines to define the "zero" point on the Y-axis (minimum ion current) and the maximum. Note that the values in the numeric boxes to the left will change as you adjust the bars. Select OK to apply the scaling to the view. Redo if necessary until the view looks correct.



Note that you can print the results at any time using the Print/Preview tool.



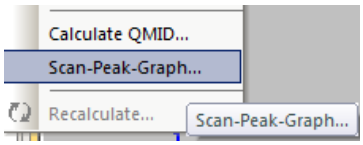
The print preview (after peak labeling explained in the next section) will look like:



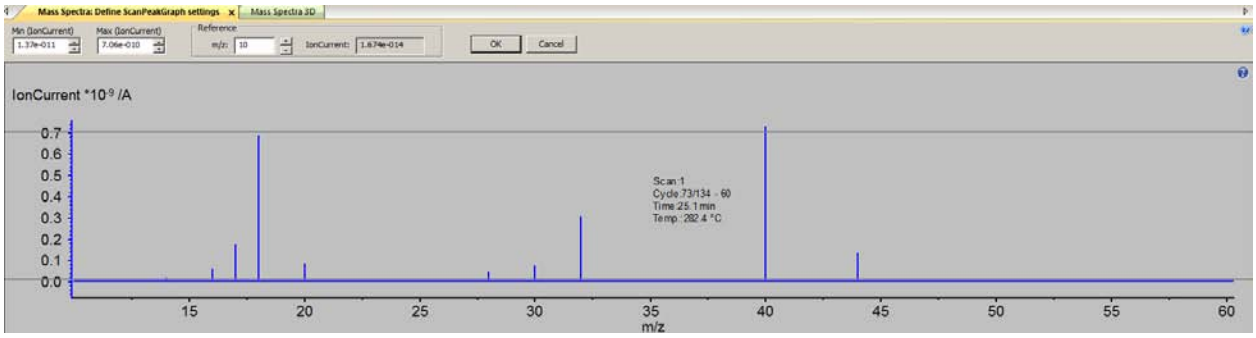
Labeling Peaks and Exporting in NIST Format

In order to label the peaks on the spectrum, a peak table must be created. This same peak table can then be exported in NIST format to allow use of the NIST library search software.

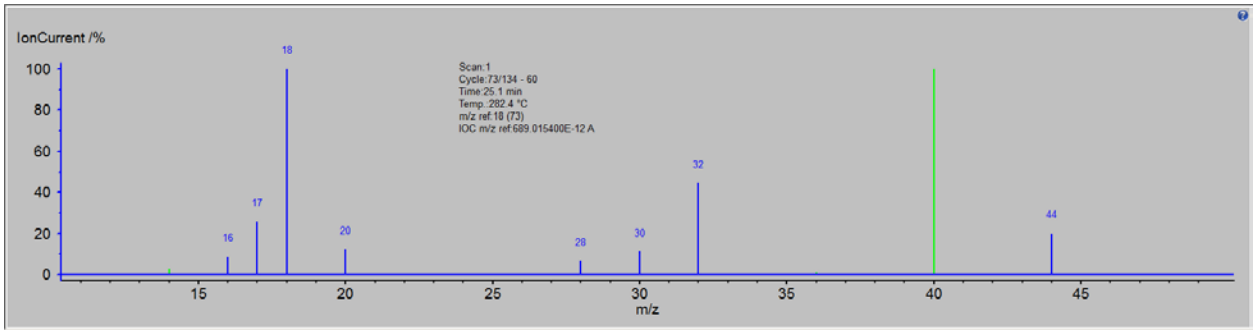
From the Evaluation pull-down, select *Scan-Peak-Graph*



Adjust the cursors to define the thresholds (min and max) for peaks to be put in the peak table. Also set the Reference m/z value. This is the Netzsch terminology for setting the base peak. In this case, set it to m/z 18.

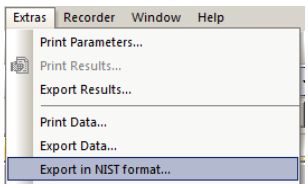


You will note that the resulting labeled spectrum is automatically un-zoomed in the x-axis. Re-zoom in the x-axis to obtain the following view. Note that ions "clipped" by your max cursor will be shown in an alternate color, and will not be labeled or put in the peak table!

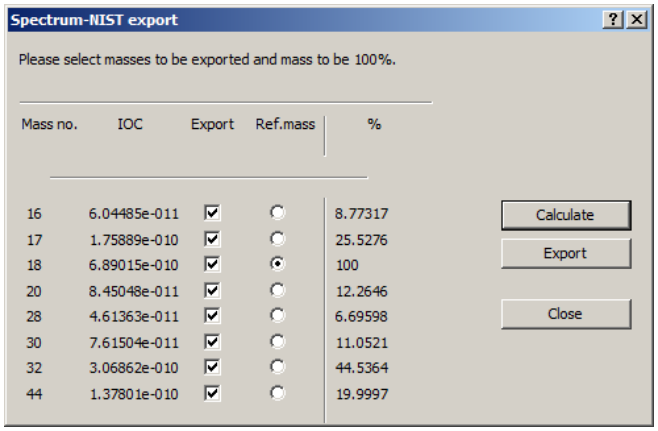


You will also note that once you are in the *Scan-Peak-Graph* program, you lose the ability to change the background cycle. It will be grayed out.

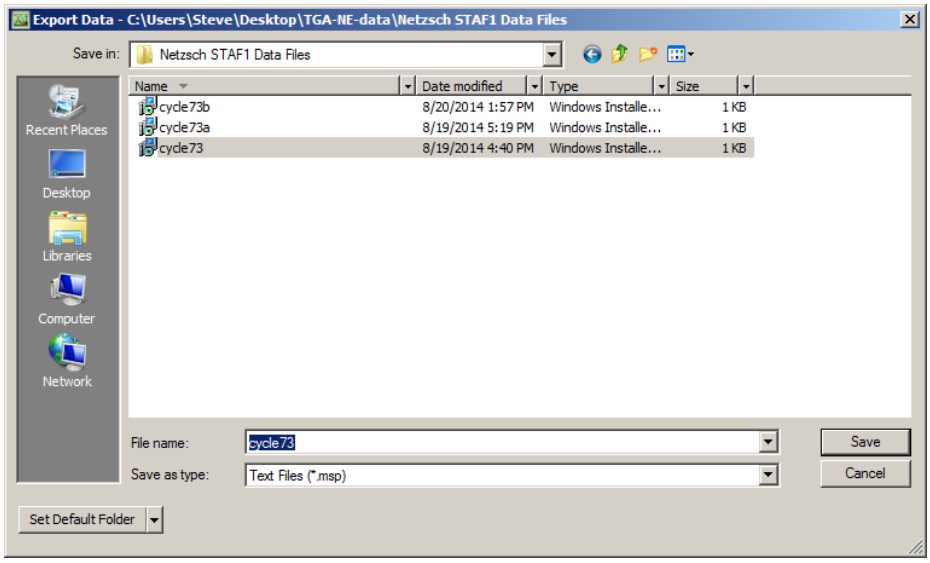
At this point you may wish to export the spectrum for use with the NIST library program. In the Extras pull-down, select *Export in NIST format…*



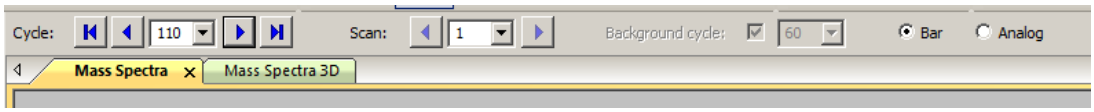
The spectrum peak table will be displayed. At this point you can de-select masses that you feel don't belong in the spectrum. For example, m/z 20 is almost certainly the double charged ion from Ar at m/z 40. For this tutorial, leave them all selected.



Select Export. A file dialog box will open. Navigate appropriately, name the file, and save it.



At this point, if you wish to view other spectra, simply move using the Cycle selection box. Note that you cannot change the background scan though. Obviously you can export these new spectra as well.

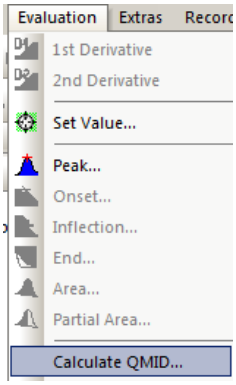


Normally you should define a background spectrum in the vicinity of the spectrum of interest. Therefore in the *Evaluation* pull-down, un-check *Scan-Peak-Graph*. This should now allow you to select a different background scan. It will then be necessary to go back into the *Scan-Peak-Graph program* to create a spectrum peak table, et cetera.

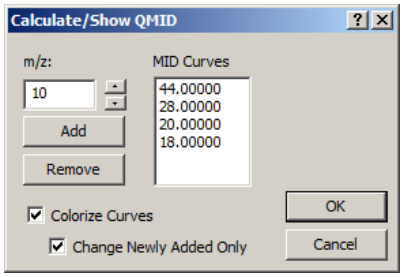
Multiple Ion Detection (Post Processing)

From the original scan-bargraph data, single-ion chromatograms can be extracted in order to help determine the evolved gases. *Note that true multiple-ion detection data must be acquired in MID acquisition mode.*

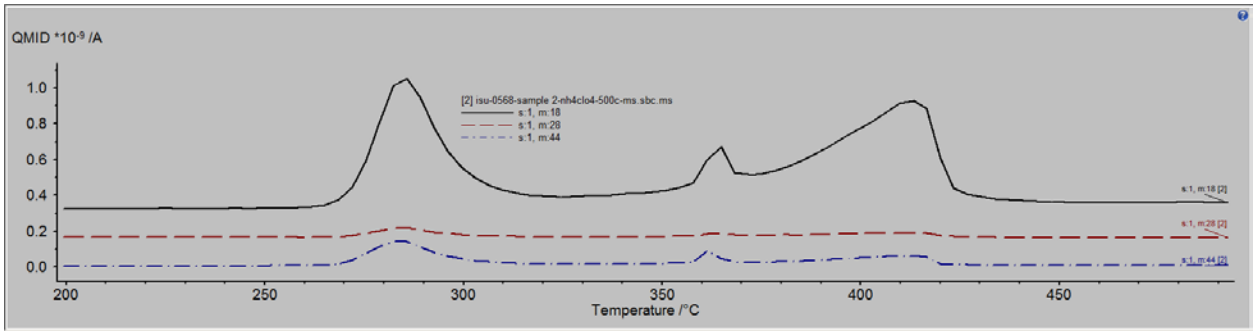
From the Evaluation pull-down, select *Calculate QMID*.



A dialog box will be displayed. Specify the m/z values you would like to monitor, and add them to the MID Curves box. Select OK. *Note: The QMID traces will be viewed in the Main view, not in the Mass Spectra or Mass Spectra 3D views*.



Select the Main view. In the browser, expand as necessary and deselect everything except the QMID ions 18, 28, and 44. Change the X-axis from time to temperature  . Zoom to show from 200 ->500 C.

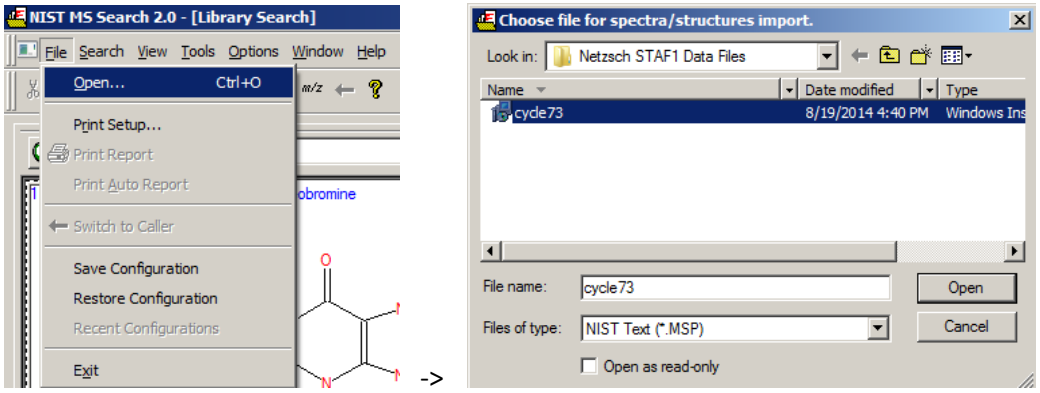


Note that right-clicking on the curves will allow you to move them up so the baselines superimpose, but it is not possible (as far as I know) to independently normalize the QMID curves in the display.

NIST Library Search Program

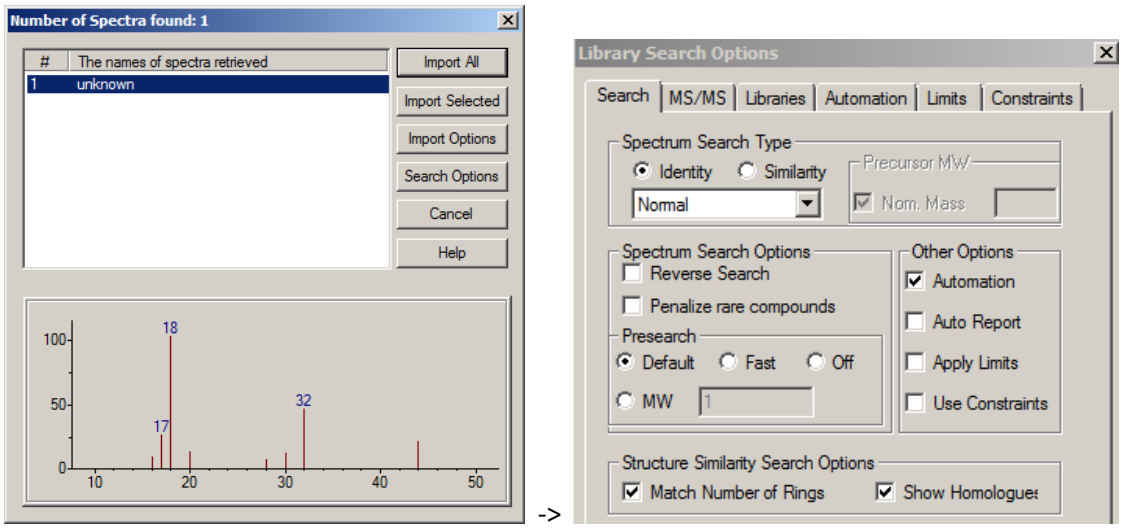
Within Proteus, create and export in NIST format all of the relevant spectra you would like to search in the library. At the desktop, select the *MS Search v.2.0* icon.

The NIST MS search program will start. From the File pull-down, select Open

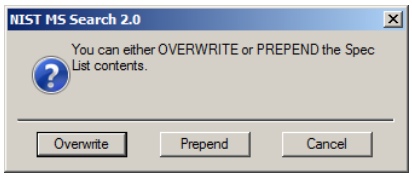


Choose the spectra files to import. In this instance we only have one in the folder, corresponding to cycle 73, with cycle 60 subtracted.

A simple-looking Import dialog will pop up. However, be aware that many important choices are available here by selecting the Search Options button.



Choose *Import Selected*. In the resulting popup, choose to *Overwrite* the Spec List contents.



The NIST search results will now be displayed.