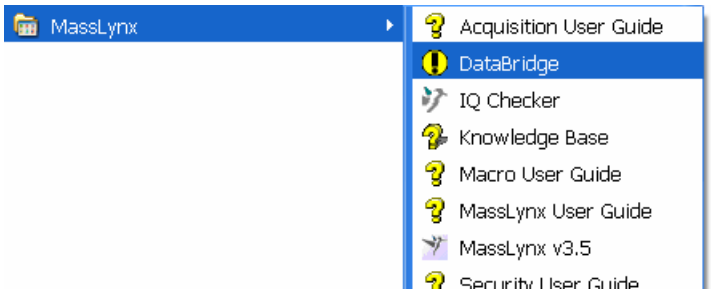
Step-by-step instructions
for creating a 3D Origin plot from a MassLynx continuum file

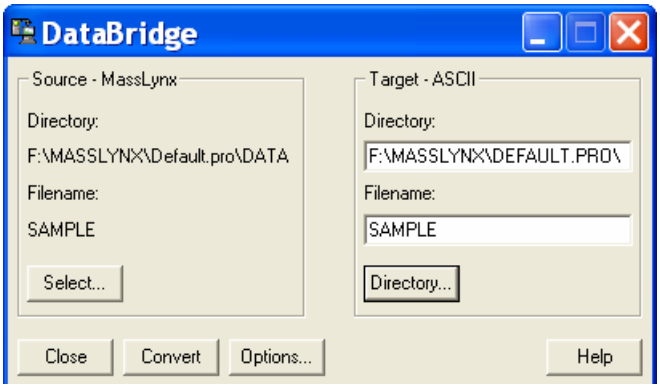
Your mass spectrum will be saved as a series of files in a folder called SAMPLE.raw (where SAMPLE is your filename).

DataBridge

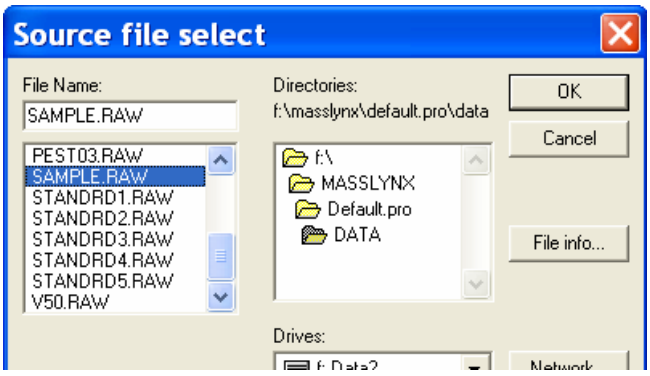
Open DataBridge:



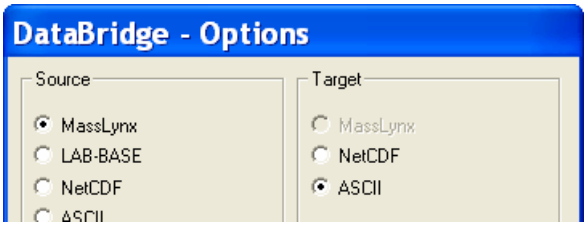
You will be greeted with the following screen:



Hit "**Select…**" and browse to your spectrum:



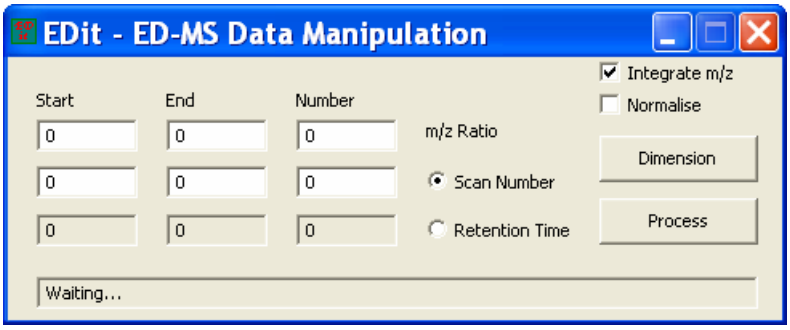
Check that under "**Options…**" the conversion is set to Source = Masslynx, Target = ASCII:



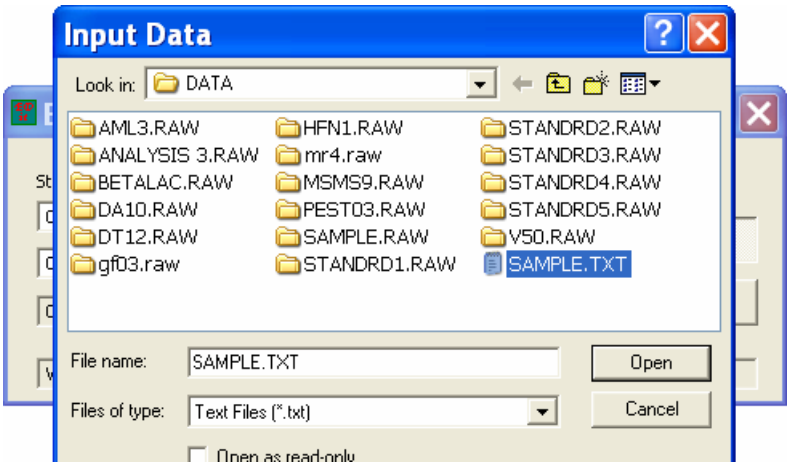
Hit "**Convert**". The file will be saved as a .txt file, which may now be treated with EDit.

EDit

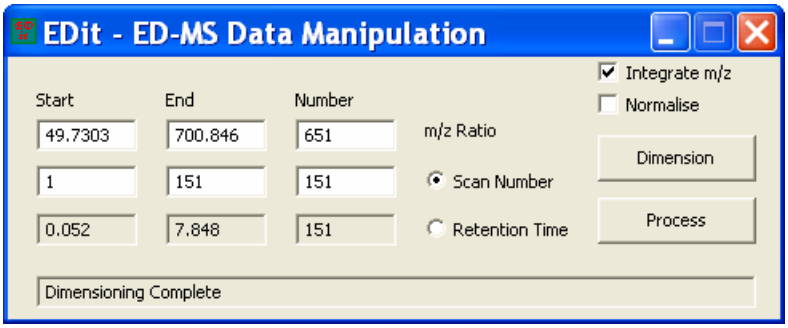
EDit may be downloaded freely as a .zip file (http://web.uvic.ca/~mcindoe/edesi.html). The file should be unzipped and saved to disk (EDit.exe). Upon running the program, users will be greeted by the following dialogue box:



To begin, hit "**Dimension**", and browse to the .txt file previously generated from DataBridge.



The program then fills out the boxes according to the data found in the file:



The top row indicates the start and end values of *m/z*. "Number" indicates the number of *m/z* units between these two values (in this case, 701 – 50 = 651). If a higher resolution than 1 *m/z* is required, increase the "Number" value accordingly (e.g. for a resolution of 0.5 *m/z* in this example, change to 1302). The second row similarly computes the number of scans – there is no advantage in increasing the "Number" setting here (you can't increase the number of scans unless you repeat the experiment) but in some cases it may be useful to lower the number (e.g. a very weak sample may have had 4 scans collected per increment in the cone/collision voltage, in which case dividing the "Number" value by 4 is necessary). Finally, the third row gives the actual retention time rather than scan number, which is useful if chromatographic information is to be manipulated instead of a variable set to change linearly with scan number (as is the case for ED spectra).

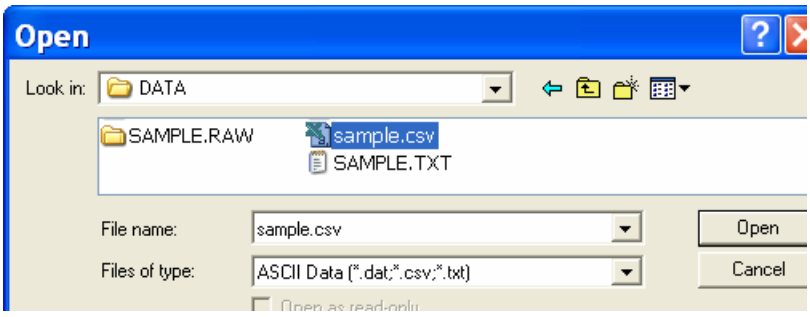
The two "Number" settings give the size of the matrix, in this case 651 × 151. Hitting "**Process**" allows you to choose the same .txt file and to perform the conversion to .csv format with the appropriate settings. Save the .csv file; it is now ready for processing using your scientific graphing package.

The "Integrate *m/z*" option sums up all of the intensity samples collected for every *m/z* within the range of the output "bin". When the *m/z* data are not equally distributed, this can result in more samples being integrated in one region (e.g. at low *m/z*) than another (e.g. at high *m/z*). This is usually the desired result, this conserves all data within the range. However, for some applications it may be desirable to divide by the number of samples collected within the *m/z* "bin", thus an averaging rather than an integrating behaviour. In this case deselect the "Integrate *m/z*" option. Note that in all cases, scans are averaged if there is more than one scan in an output "bin".

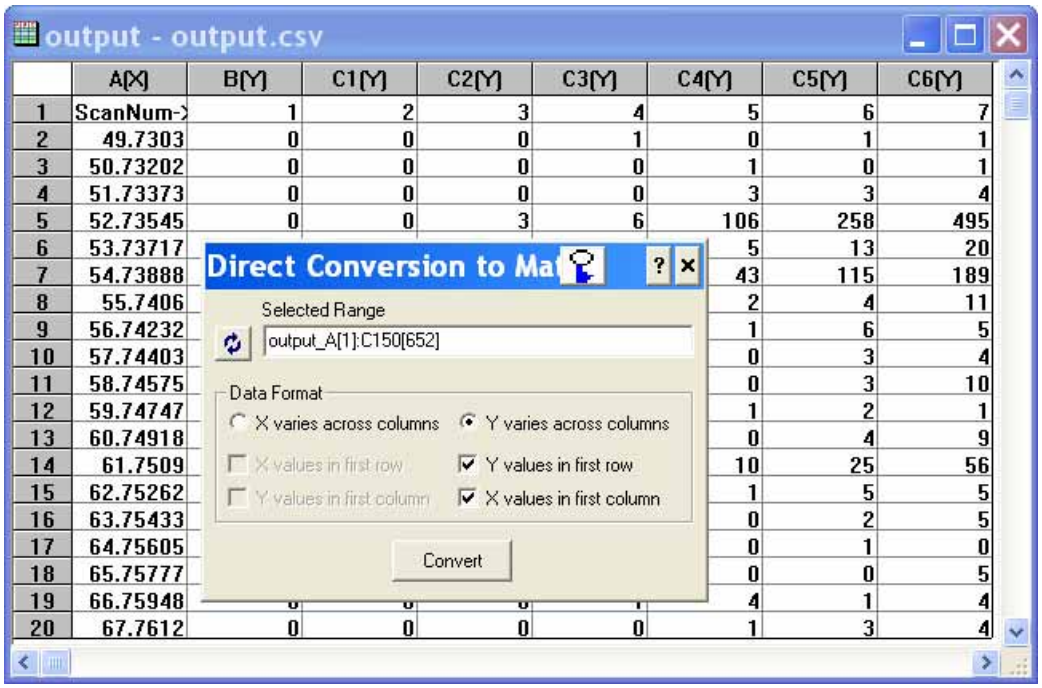
The "Normalise" option simply scales all of the output data to the highest (absolute) value observed in the data (after integration or averaging described above). Thus the data lie on a known scale from 0 to 1.

Origin

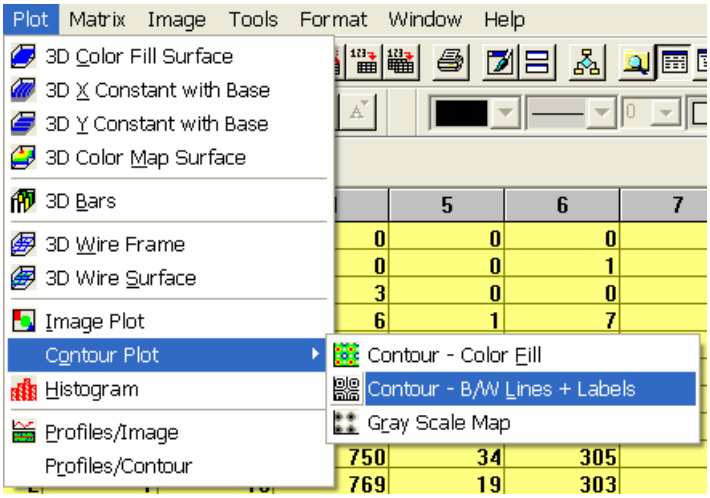
Click on "**File**", and "**Open…**". In the first dialog box under "**Files of type:**" choose "**ASCII Data (*.dat, *.csv, *.txt)**". Browse to the .csv file you saved as output from the EDit program:



The open file must be converted into the special Origin matrix format in order to plot 3D graphs. Select "**Edit**", "**Convert to Matrix**" and "**Direct**". Click on the radio button for "**Y varies across columns**" and check the boxes for "**Y values in first row**" and "**X values in first column**":

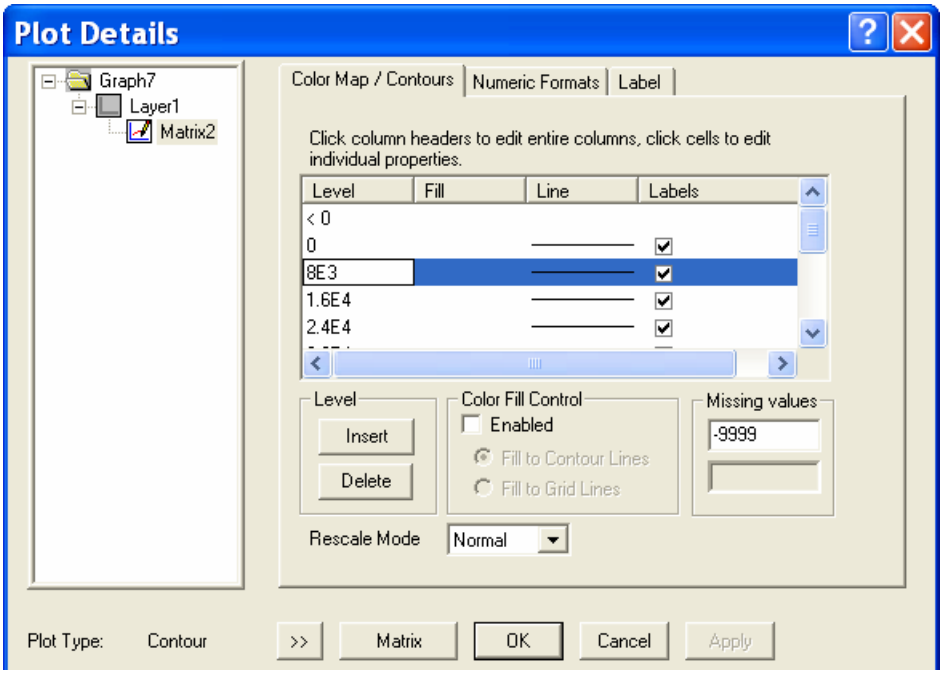


The resulting matrix (the data appears with a yellow background) may be plotted in a variety of styles, but the best place to start is probably a simple contour map:



The initial plot will probably appear nonsensical until Speed Mode is switched off (the matrix is usually a large one). Go to "**Format**", "**Layer…**", go to the "**Size/Speed**" tab and uncheck the box labelled "**Matrix data, maximum points per dimension**".

Origin automatically assigns contour lines to particular values; like all other features of the graph, these may be altered to suit. Generally, users will want to enhance the lower intensity peaks. Double-click on any peak in the spectrum, and you will be greeted by the following dialog box:



Double-click on the value under "**Level**" and enter a smaller value. Other contour lines may be added, subtracted or adjusted to suit the desired picture. Maximising real signals while leaving out noise is the primary goal.

Relabel the *x* axis *m/z*, and the *y* axis with whatever parameter is appropriate, e.g. cone voltage, collision voltage, time, etc.