# Melissa Trainer

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Online site for IGOR-based routines used to analyze atmospheric QMS data - contributed by Melissa Trainer.

# Recommended Analysis Procedure using these IGOR routines

Media:MGT_IGOR_Analysis_Procedure.pdf?

# Igor scripts for SAM data anaylsis

**Deadtime Correction**

Media:Deadtime_mgt.ipf

This IGOR routine is used to perform a deadtime correction on any SAM data wave. There is an option to select the electron multiplier used in the experiment, since that determines which deadtime coefficients are most relevant. The deadtime coefficients are parsed as discussed in the following file from Heather Franz:
Media:Franz_SAM_deadtime_coeff_20120808.pdf

To use these IGOR routines (and the ones on Mike Wong's page) you need to use python scripts to export SAM data into a delimited text file. *For instructions on how to do this (using gcms.py) for a range of m/z values, see the tutorial below.* This data is then loaded into IGOR through the Data --> Load Waves --> Load Delimited Text menu item. If the header information is removed from the file exported via gcms.py, then IGOR will find the column headings and automatically name the waves.

TUTORIAL: Exporting data using python

Run through the Command terminal window.

1. In HOME directory, access data folder of interest. It will probably be located in `<home>`/SAM/gse/data

2. To export chromatograms and save as text file [where "filename" is your chosen file name], either for a single value (X) or a range of m/z values (X-Y), type:

"gcms.py X > filename.txt" OR "gcms.py {X..Y} > filename.txt"

3. This will place .txt file in the data folder (use different extension, such as .xls, to suit needs). The data will be in time (s) and counts (cps) per m/z charge. It is tab delimited.

4. To export bands, either a single (B) or range of bands (B-C), and save as text file type:

"gcms.py -b B > filename.txt" or "gcms.py -b {B..C} > filename.txt"

[Note for windows, the "{X..Y}" will not work. Either list the m/z values you want one by one, or export all by just running gcms.py.]

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**Calculate Average Ratio Fit and Error**

Media:Calculate_average_fit.ipf

This IGOR routine is used after the makeratio.ipf to get the count ratio of two m/z values (see Mike Wong's page ). This routine will calculate the average ratio, and will use a fitting mask to only include certain points in the fit (ex// exclude background regions). To use this routine you need to have a fitting mask wave prepared, with the same number of points as the ratio wave. Fitting mask values should be "1" for points you want to include in the fit, and "0" for points to exclude. The routine results will print to a new table, giving the average value, standard deviation, standard error of the mean, and number of fit points.

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**Load and average Fractional Mass Spectra**

This is an IGOR routine that will take data exported from gcms.py (must include fractional scan points) and generate averaged mass spectra over specific time regions. Can be used to create "Background" and "Sample" mass spectra for analysis. There is a how-to pdf included in addition to the IGOR procedure file:

Media:AtmTeam_Fractional_Spectra_HowTo.pdf

Media:Fractional Load and Average.ipf

**Fractional Mass NEW VERSION:**

(2012-09-06 --mikewong) In addition to calculating a wave for the average spectrum, it also calculates waves for the standard deviation at each fractional mass point, and the number of samples used in the average. **Note:** Standard deviation is not necessarily the same as uncertainty, unless the signal is constant in time and all the variation is due to noise.

Media:Fractional_Stats.ipf

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