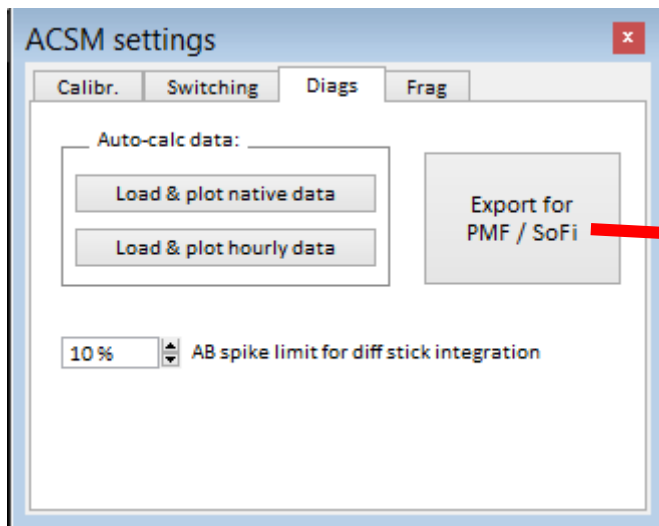


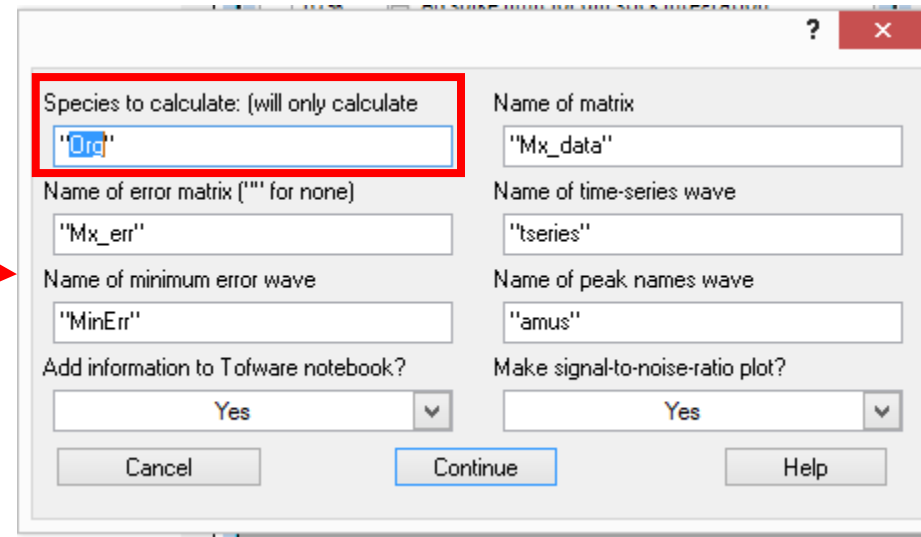
TOF-ACSM PMF/ME-2 Error Calculation

Input needed for PMF/ME-2

- Data Matrix (Organic stick mass spectrum is typical for ACSM)
- Error Matrix (Precision error)
- Time-series
- Data labels (amu wave)



You need to enter species



How to determine the error matrix

Poisson (counting) statistics:

$$e_x = \sqrt{x}$$

In the ACSM we “count” ions:

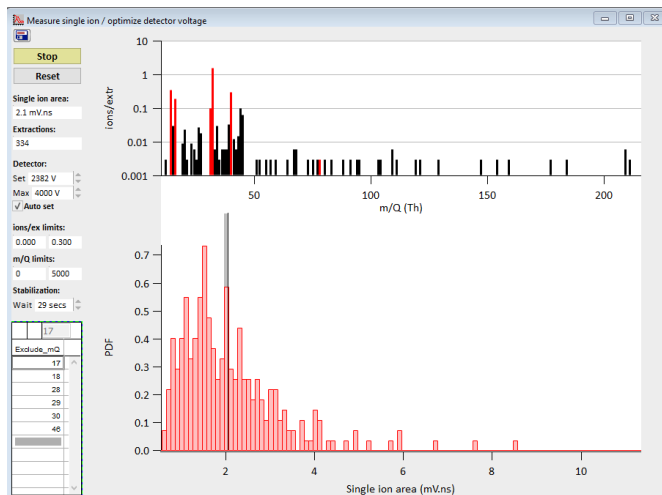
$$e_{ions} = \sqrt{ions}$$

BUT – not all ions are exactly the same intensity, so

$$e_{ions} = \alpha \cdot \sqrt{ions}$$

α is the convolution of a Gaussian with the measured single ion distribution

Measured for TOF-ACSM this is 1.2



Allan, et al., *J. Geophys. Res. – Atmos.*, 108, D3, 4019, 2003.

How to determine the error matrix (cont.)

ACSM measurement is a difference (D) between a measurement of sample (S) and of background or filter (F):

$$D_{ions} = S_{ions} - F_{ions}$$

The error in a difference is sum in quadrature of difference terms:

$$e_{D,ions} = \sqrt{e_{S,ions}^2 + e_{F,ions}^2}$$

From last slide we know:

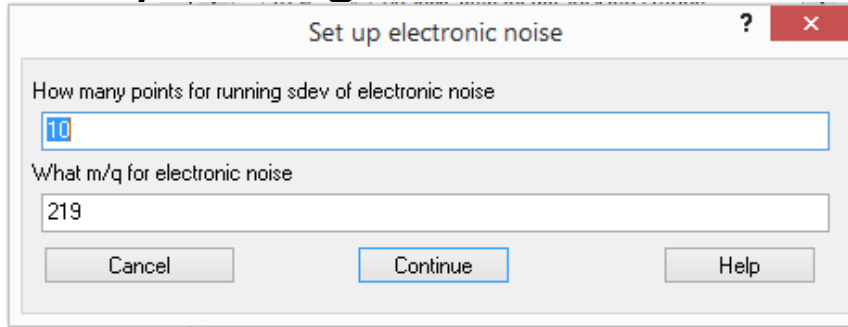
$$e_{S,ions} = \alpha\sqrt{S_{ions}} \quad \text{and} \quad e_{F,ions} = \alpha\sqrt{F_{ions}}$$

Thus:

$$e_{D,ions} = \alpha\sqrt{S_{ions} + F_{ions}}$$

We also add an empirical estimate for “electronic” noise

This is done by taking the standard deviation of the measured “signal” where we don’t expect any real signal.



*If either text box is set to zero, we skip this.
You may want to skip this if you know you have
real signal at high m/Qs, but your errors will be
underestimated (Q/Qexp will be large in PMF).*

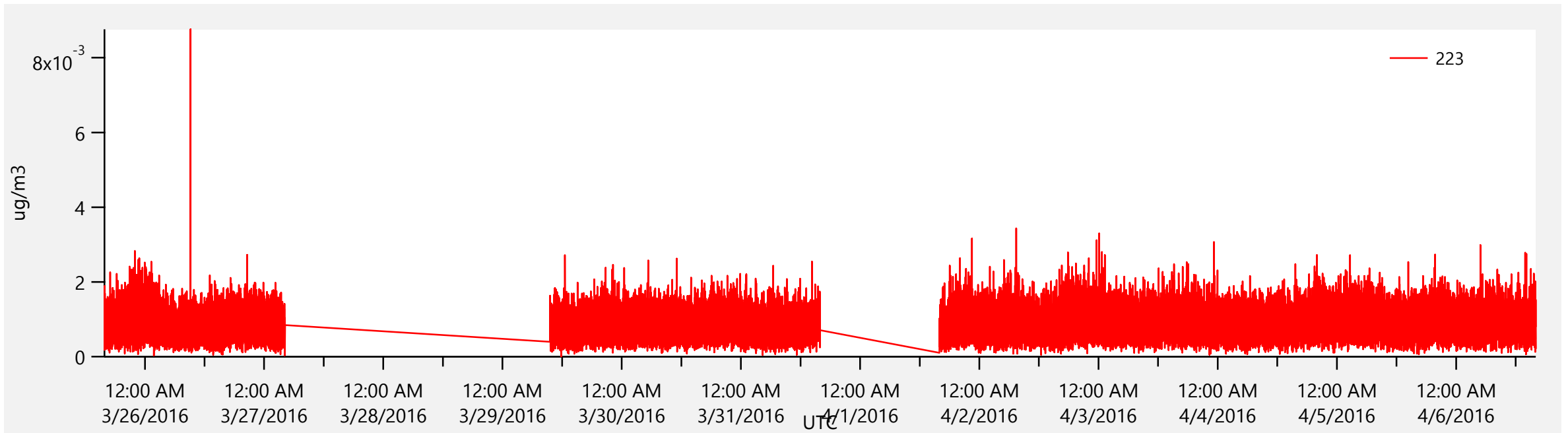
We have electronic noise in both sample and filter data so:

$$e_{D,elec} = \sqrt{e_{S,elec}^2 + e_{F,elec}^2}$$

Then this error adds in quadrature with counting error:

$$e_D = \sqrt{e_{D,ions}^2 + e_{D,elec}^2}$$

For example, for the INERIS instrument at m/Q 223. Not much real variation, so standard deviation is reasonable estimate of noise.



After we've calculated the error in ion counts

- Apply frag table
 - Sum in quadrature for these addition and subtractions.
- Optionally truncate the MS
 - Typically not much chemical information beyond ~100
- Optionally convert to $\mu\text{g}/\text{m}^3$
 - RIE and CE are applied per the batch table
- Optionally apply airbeam correction
- Tofware saves out the data as an .itx file for easy loading in to PET or SoFi

You need to enter species again

Setup the data

Species you calculated	Name of data matrix
"Orc"	"Mx_data"
Name of error matrix	Name of time-series wave
"Mx_err"	"tseries"
Name of minimum error wave	Name of peak names wave
"MinErr"	"amus"

Cancel Continue Help

Pick what to save out

Maximum m/Q to retain

100

Convert to ug/m3

Yes

Apply airbeam correction)

Yes

Cancel Continue Help