Peak Width and Peak Shape...

Pete DeCarlo

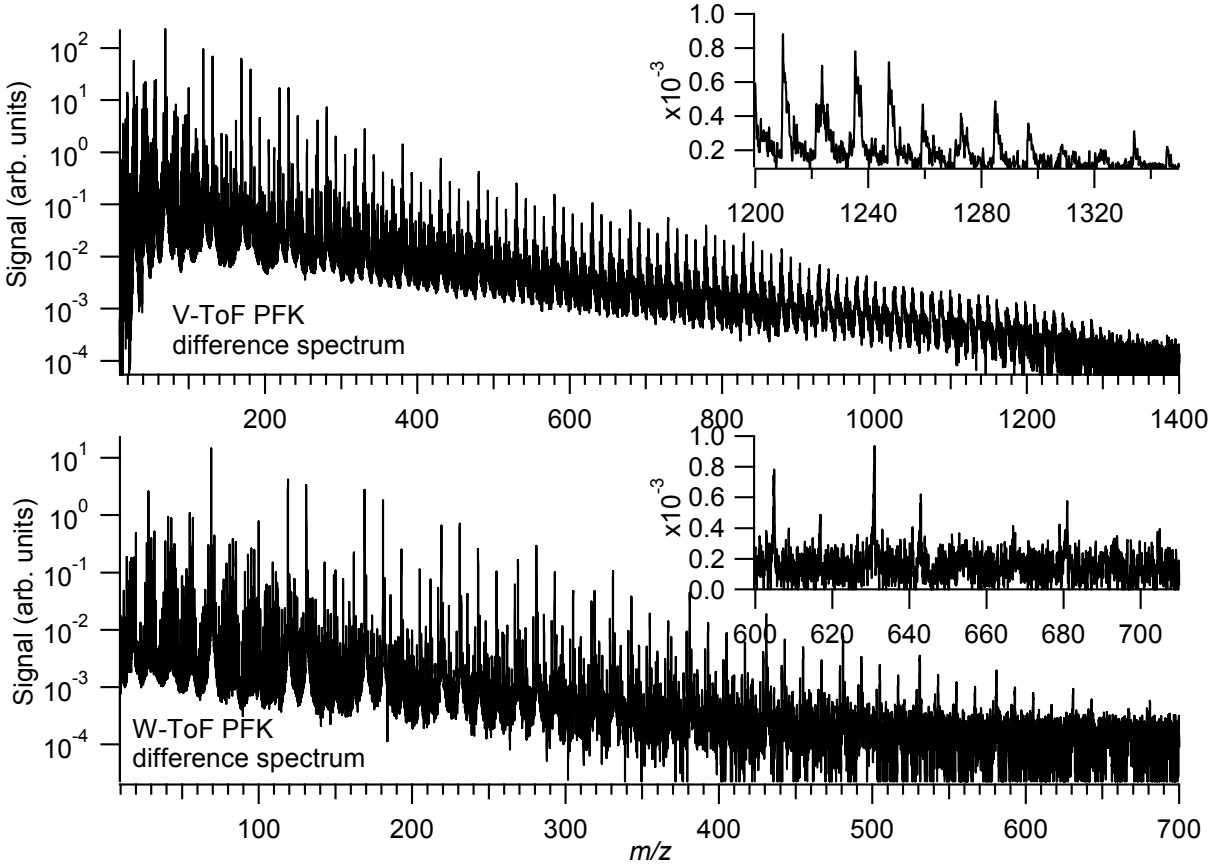
2009 AMS Users Meeting

m/z cal comments

- Center of mass of peak - Not peak center is “proper” metric
- Peak maximum introduces a little error, but more robust when there is small interferences (think N^+ and CH_2^+)
- Gaussian model is ingrained into sqrl/pika
  - m/z cal, peak width and peak shape functions.

PFK spectra...

Figure S-1. Spectra of PFK in both V and W modes of the HR-ToF-AMS. Note the *m/z* axis difference. The V-Mode data show detectable signal up to *m/z* 1300, whereas the W-mode's lower sensitivity results on detectable signal up to only *m/z* 700.



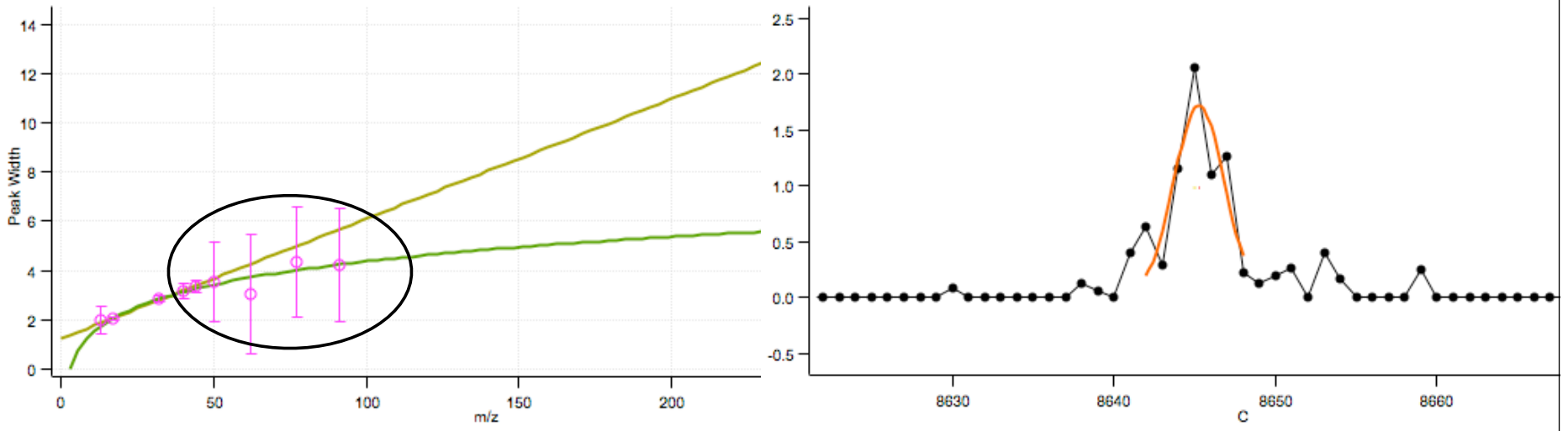
HR-instrument paper Supplementary info

Before you start...

- Make sure your m/z cal is reasonable
- If not, there's not much reason to proceed.

- Peak shape and width are independent of the m/z cal, but all must be good for PIKA to work properly.

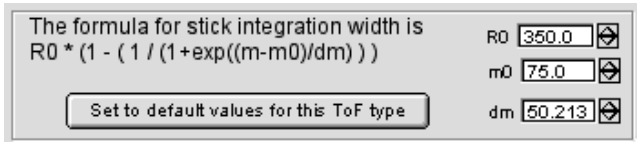
Peak Width



Low Signal to Noise Ions tend to have Smaller Peak widths.
Diagnose this with Error Bars

Linear Fit is probably better here

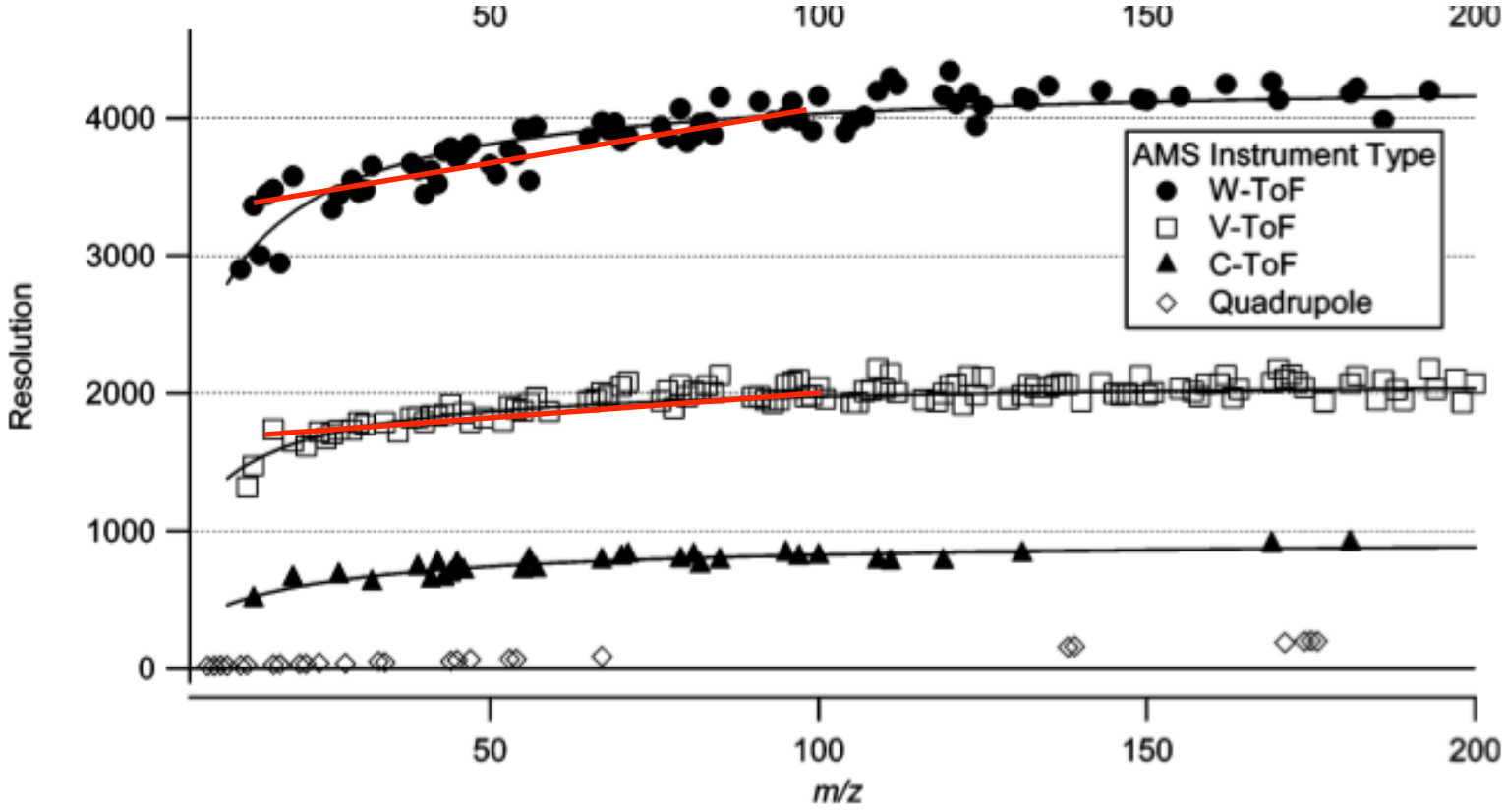
Linear vs Power Law?



The formula from the "baseline" panel is the appropriate function to use. Accounts for SI width and TOFMS Resolution

The parameters need to be changed to correctly predict the **resolution** not the stick integration area

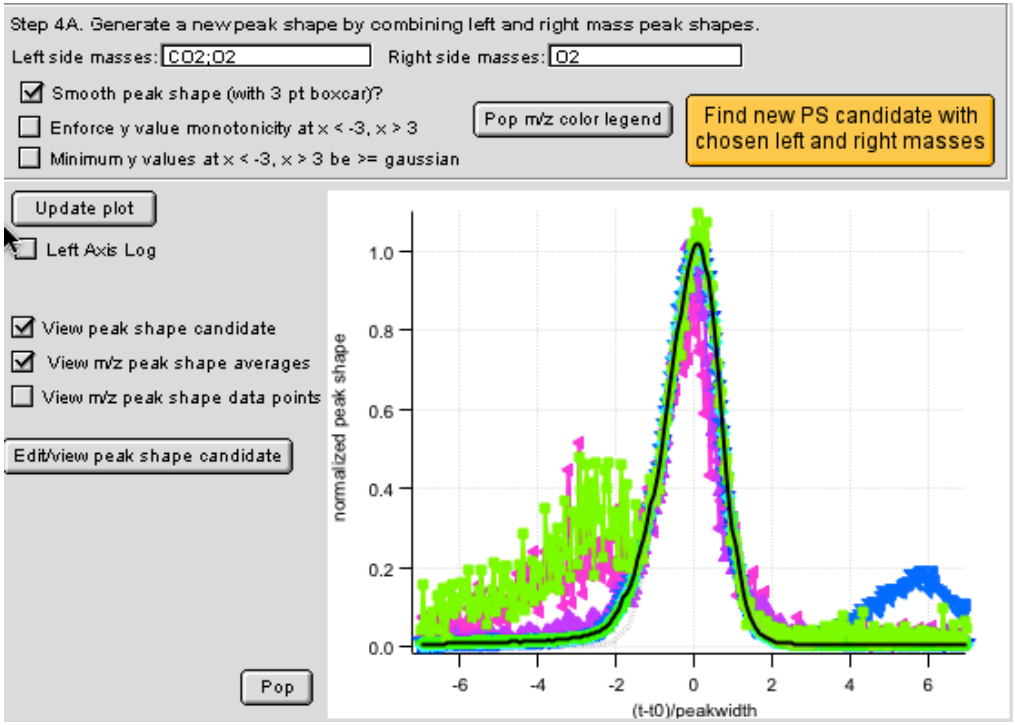
Formula applied to data



Use of standard?

- Using Fluorinated compounds one could check this with better S/N
- Use this to "guide" fits for later datasets
- Use this to "guide" peak shapes for later datasets
- Changes to TPS voltages will change these parameters so standards will have to be rerun with each change to TPS voltages
- Will require some testing and implementation by users.

Choosing a Peak Shape



a few good left side ions

O_2^*, CO_2^{**}, SO

a few good right side ions

O_2, OH, C_7H_7

Bottom line is to get clean high S/N ions with no interference. Also you need to have your peak width right

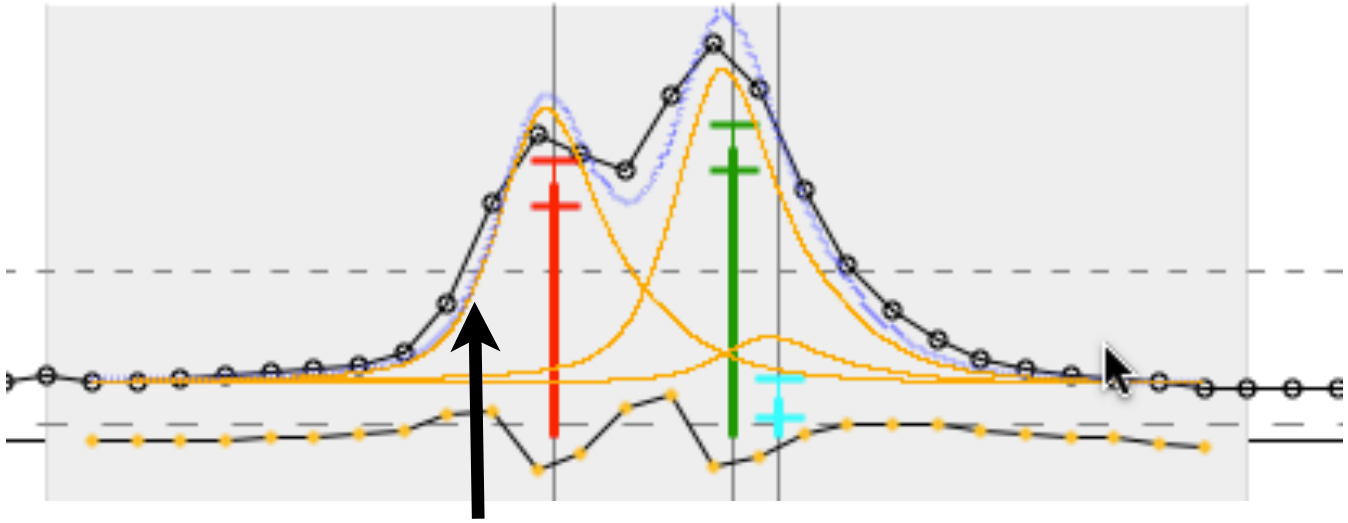
* can be problematic with lots of Sulfur

** Need to add to ion list defaults

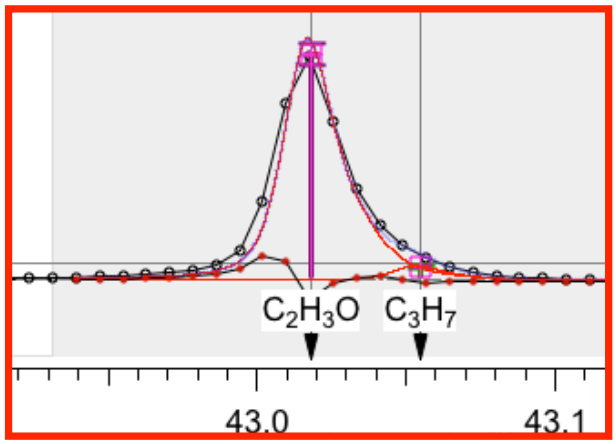
Diagnostic issues

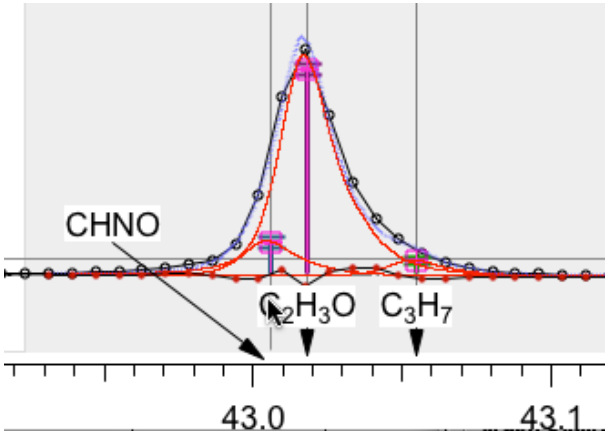
- Left edge check with e.g. SO^+ fragment
- Right edge check with e.g. $C_4H_9^+$ fragment
- Do V and W mode "agree"

Left Edge - SO+



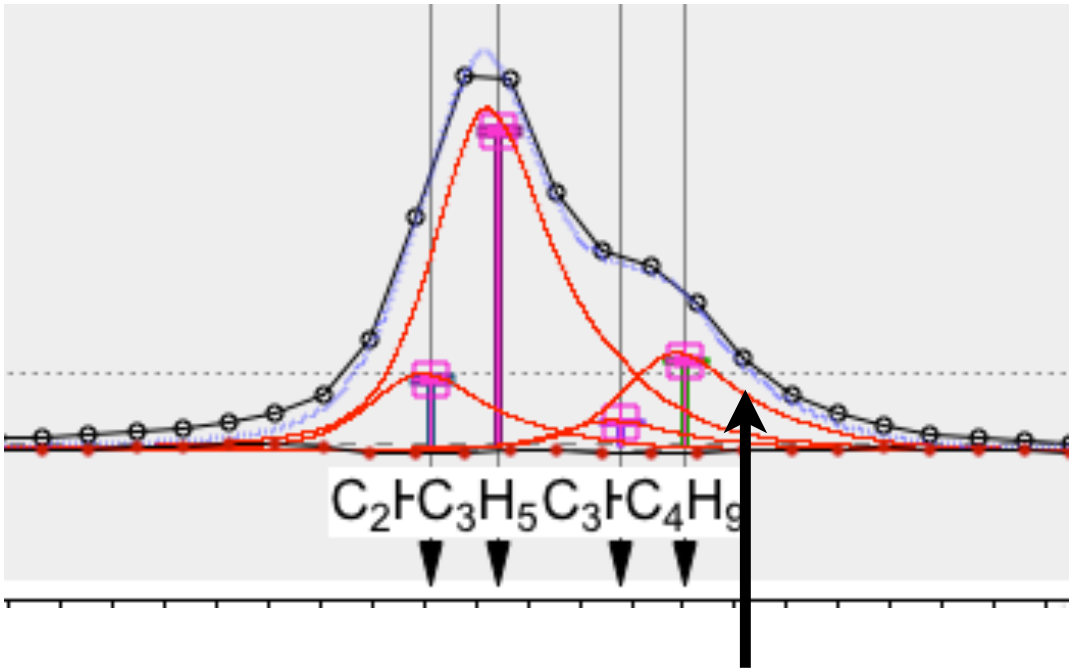
Not fit well - will cause "issues"





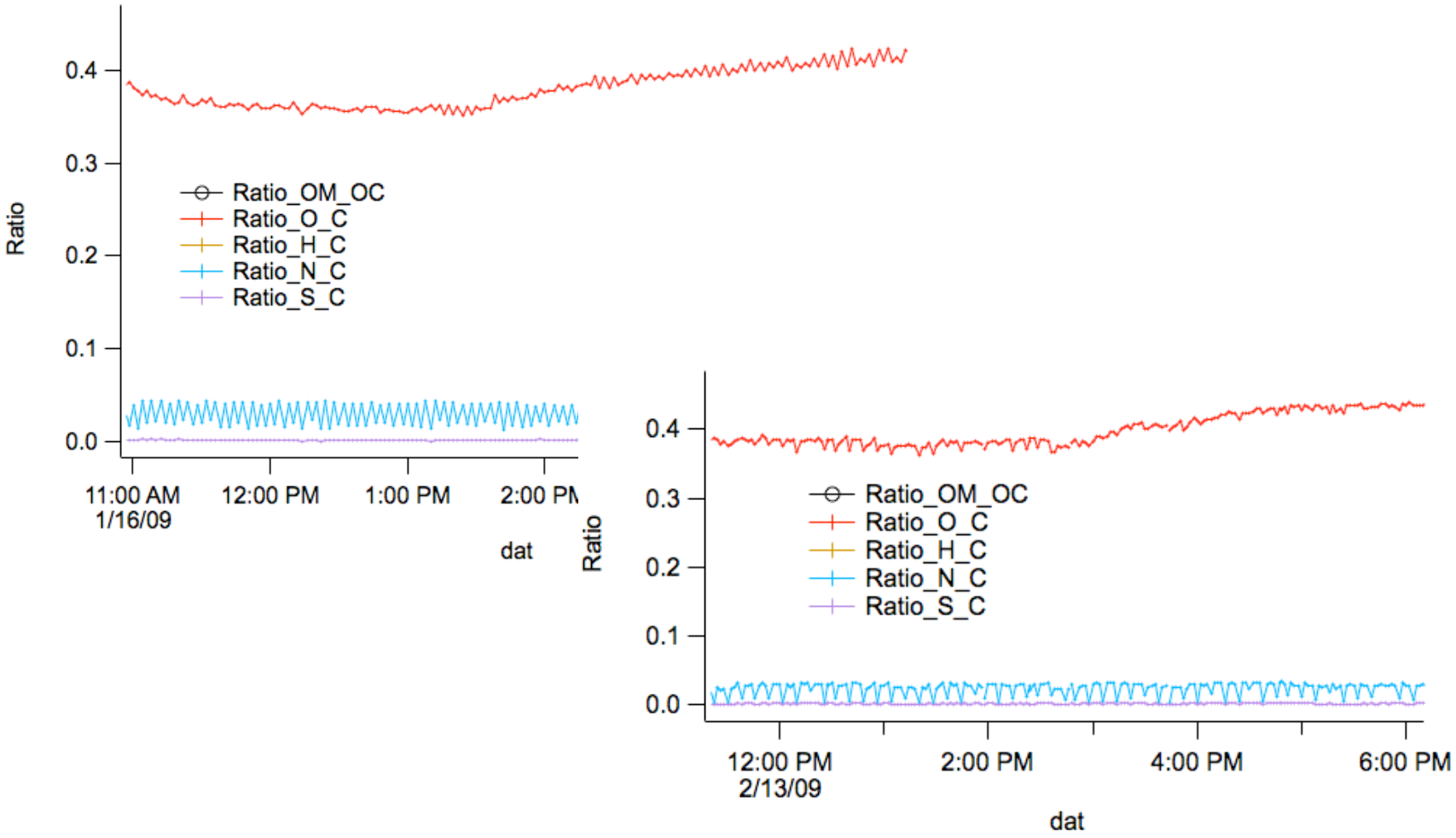
Which One?

Right Edge - $C_4H_9^+$



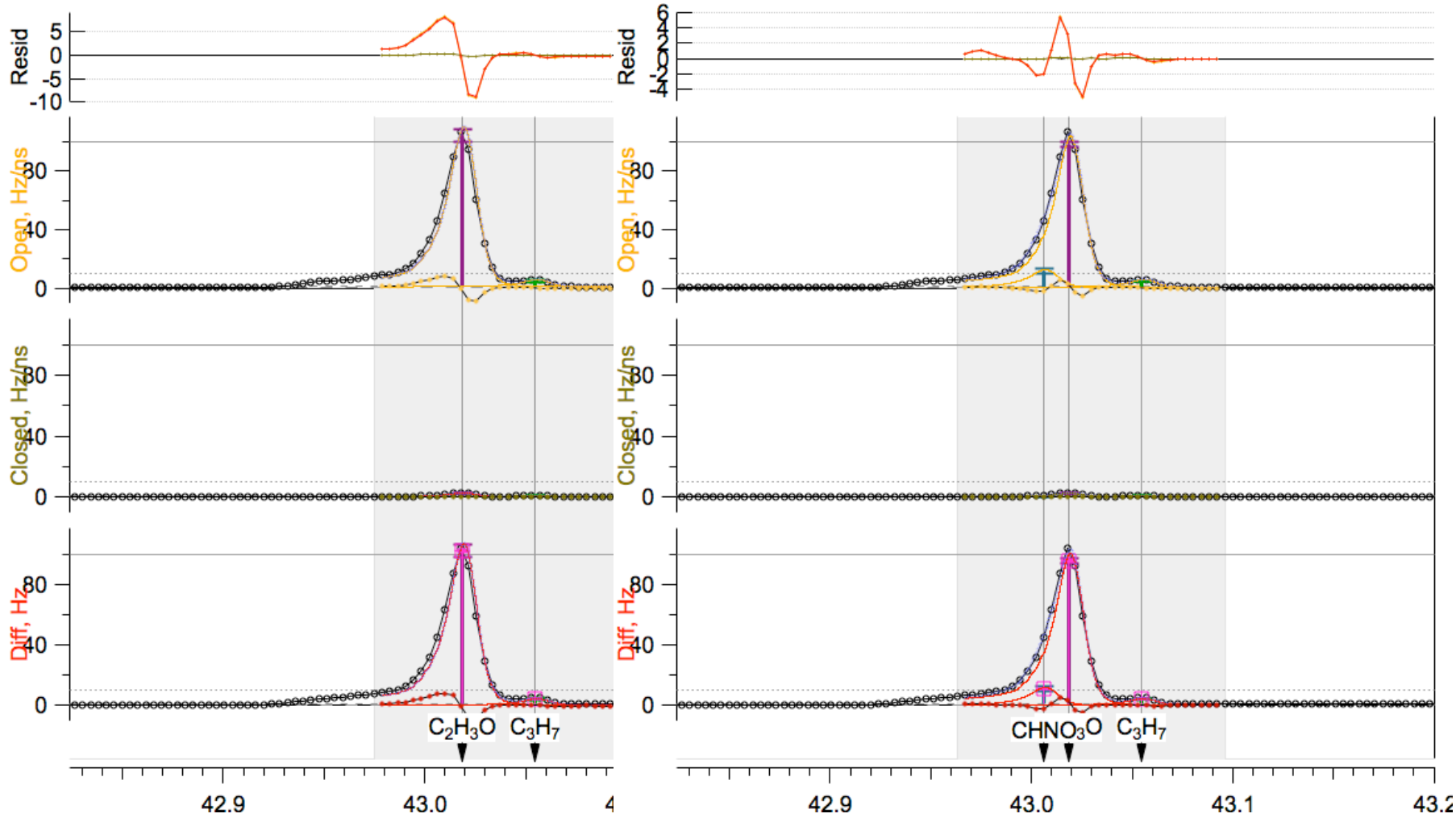
Pretty good

V - W Differences

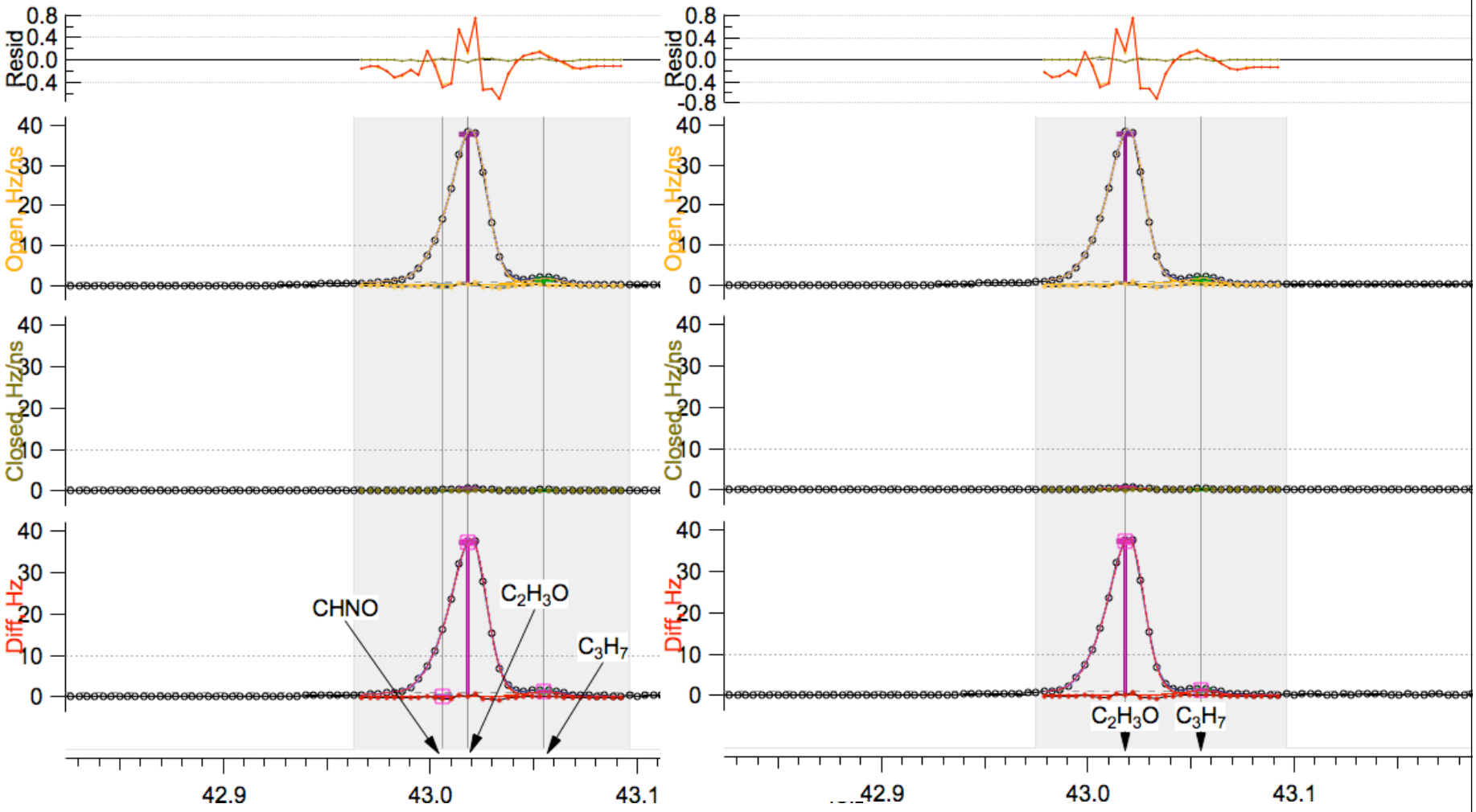


Tuning is important

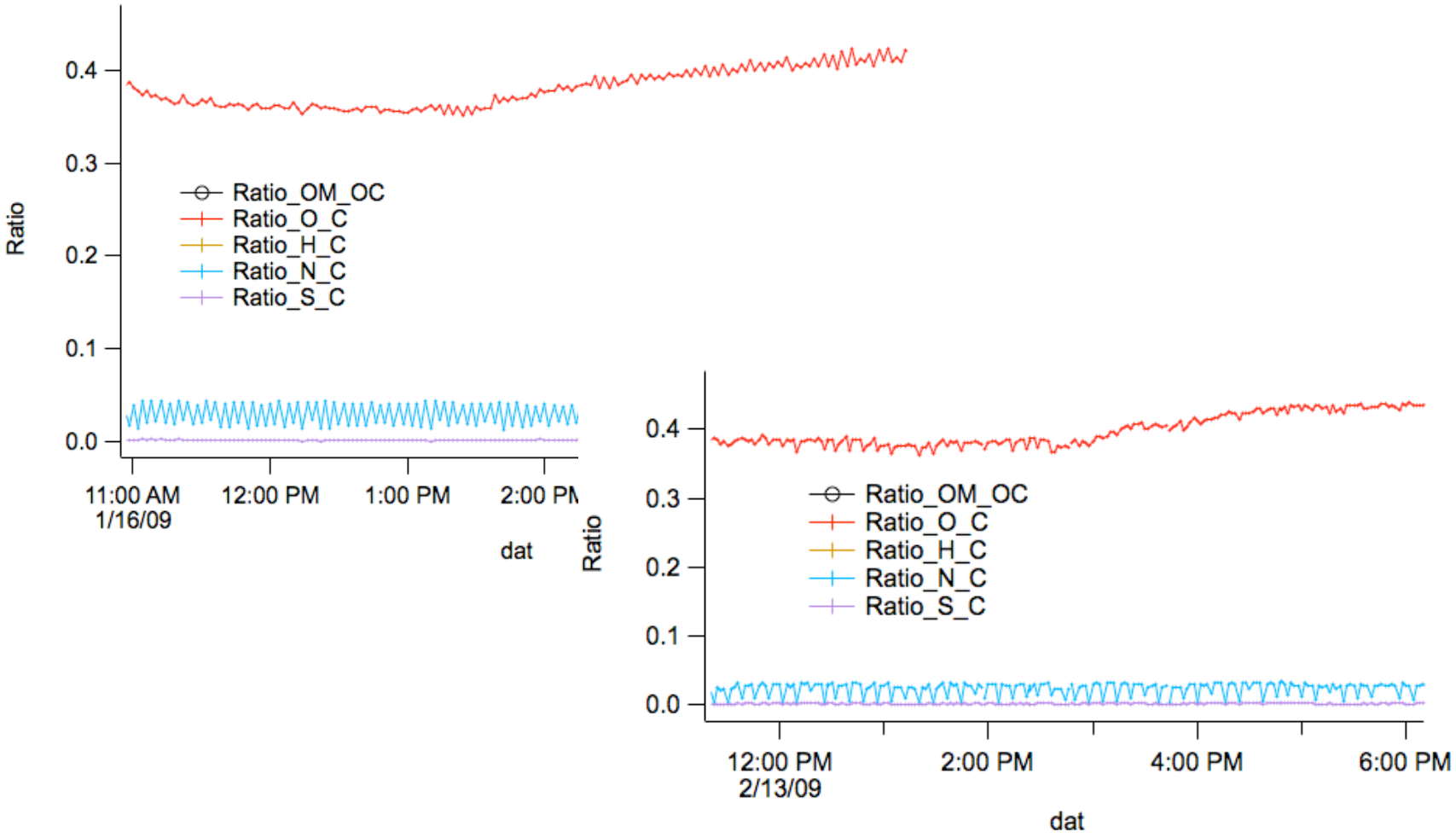
N-Fragments at m/z 43? W



W-Mode 43


Resid
Open, Hz/ns
Closed, Hz/ns
Diff, Hz
CHNO
C_2H_3O
C_3H_7
42.9
43.0
43.1

V - W Differences



Summary

- m/z cal, peak width, peak shape are ALL critical for PIKA to work properly
- Peak width and shape need high signal, isolated ions for good determination
- CH and CHO ions are easier to determine well - be extra OCD if you want N containing ions
- For a variety of reasons, sometimes you have to just accept that your data is not good enough for HR analysis in PIKA