

# A story of unexpected HRNH4 inaccuracy

V mode, overall low loadings

Pika 1.15P

Donna Sueper

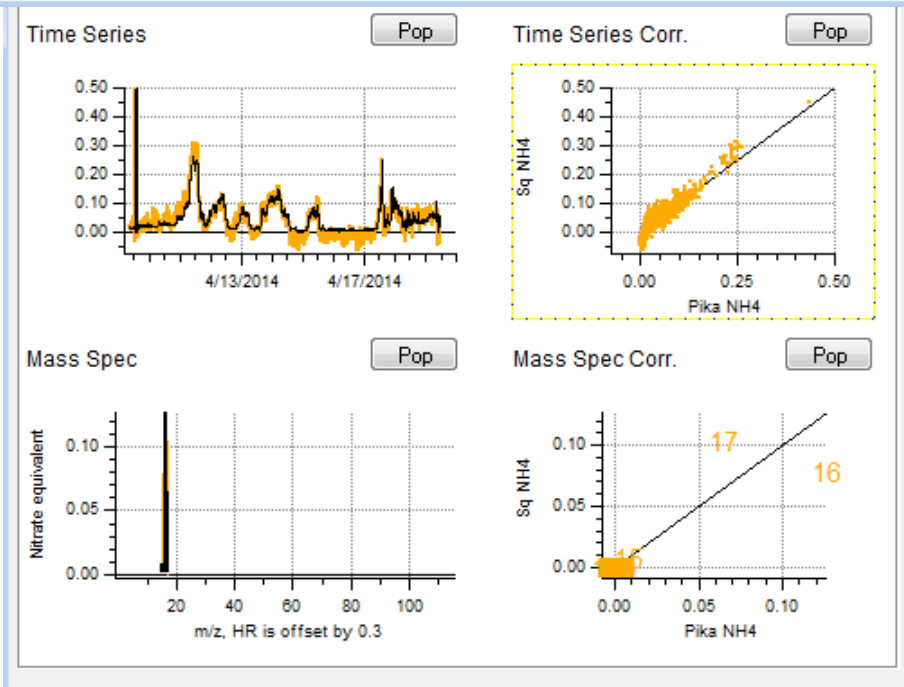
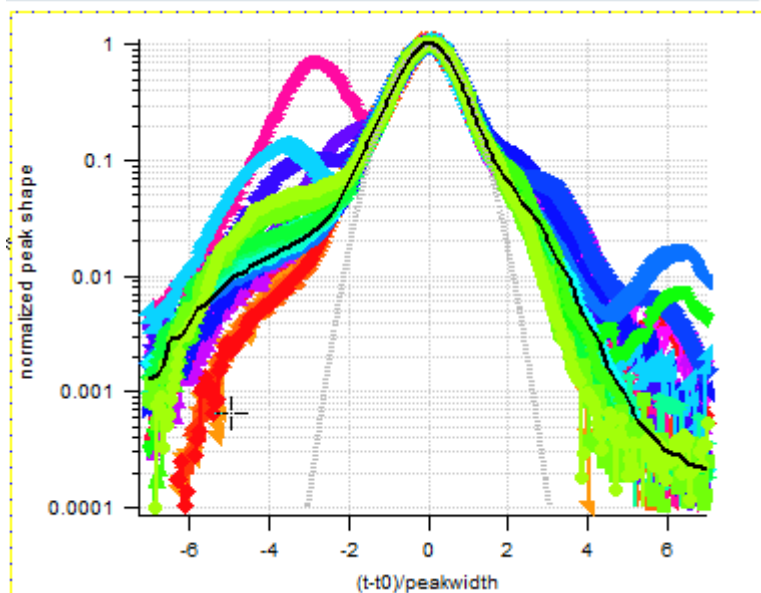
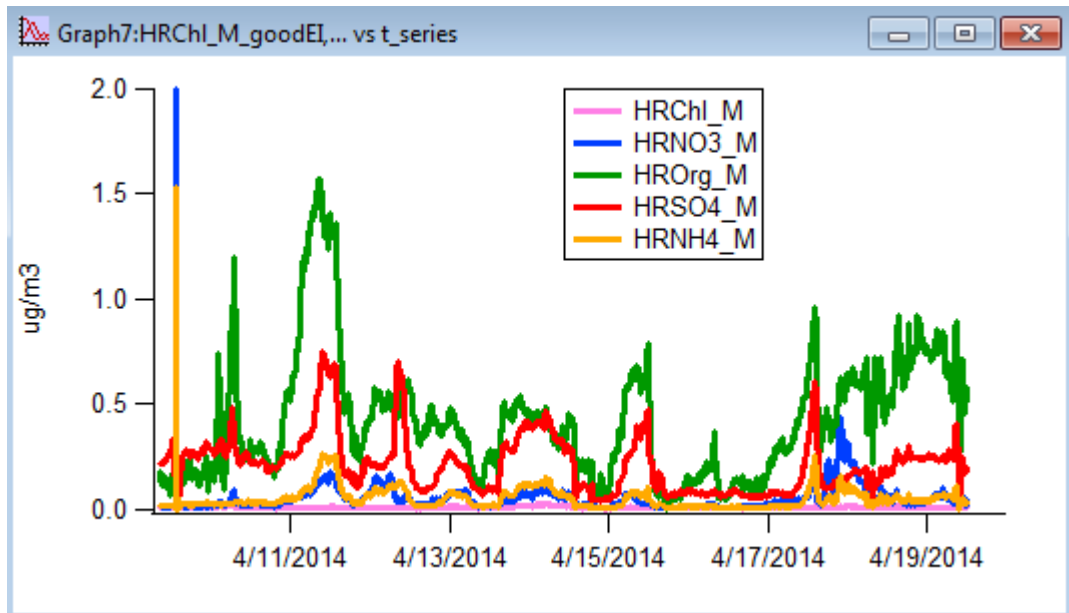
Standard analysis

Default HR ion list

HRStickOMinusC data set

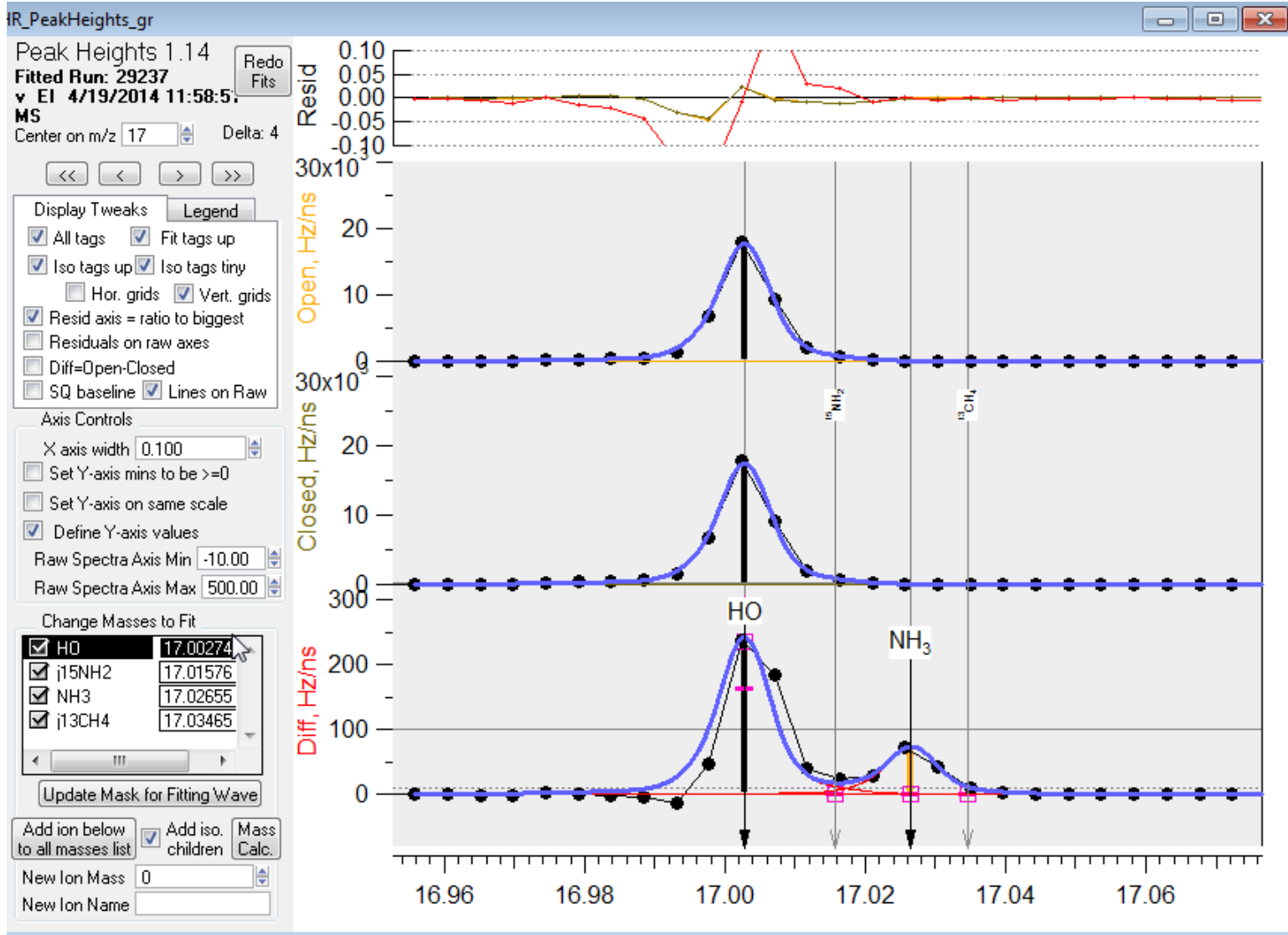
Peak shape seems fine

HRNH4 appears to have no problems, right??



(Cue music from 'Jaws')

Intro Pika Plot at m/z 17. Y scales for Open and Closed are 100x larger than of Diff axis.

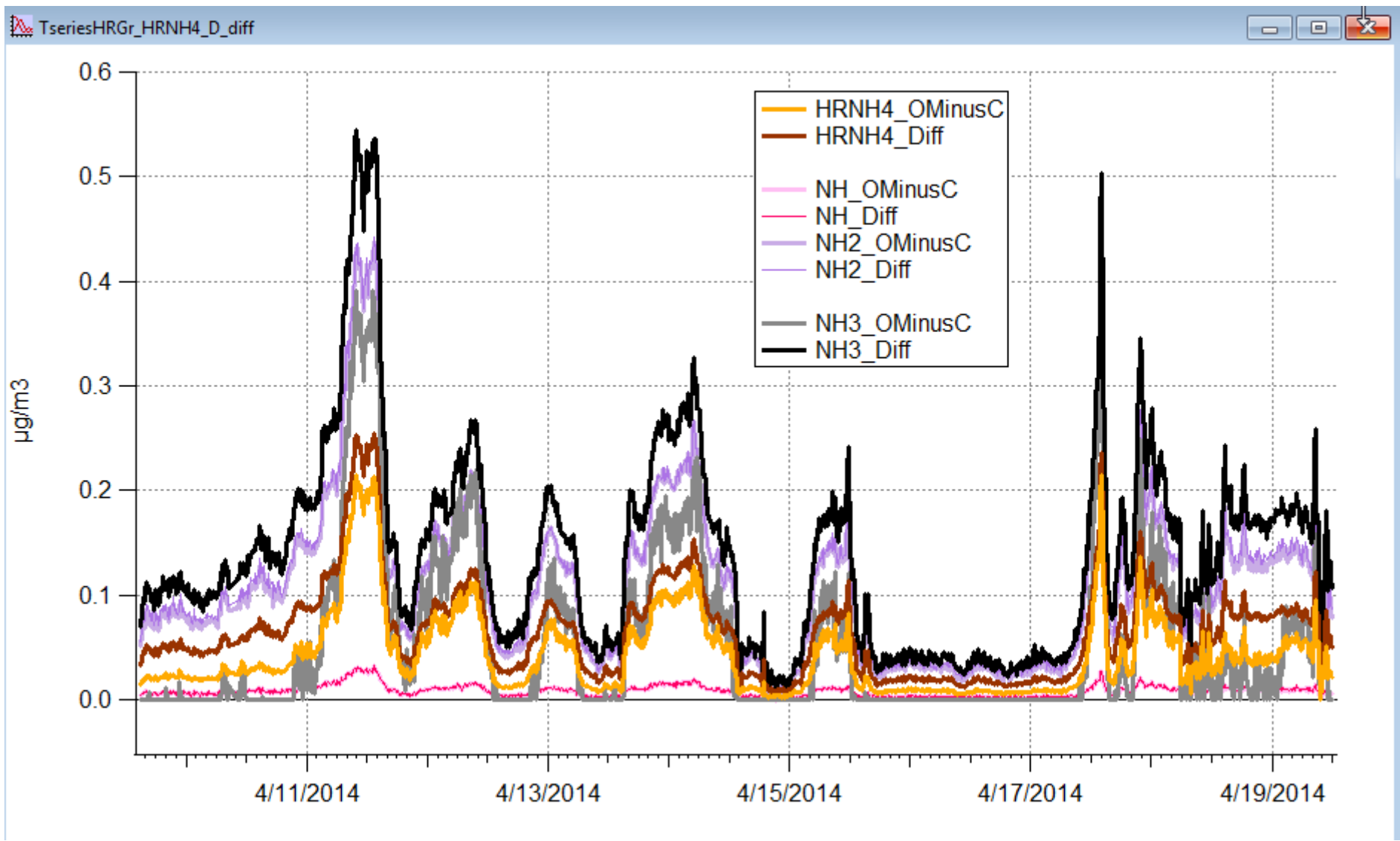


In this data set OH is a dominant peak. It seems that OH and NH3 are separated enough to be resolved... but only in the diff data set!

(More intense 'Jaws' music)

# NH3 Problem!!

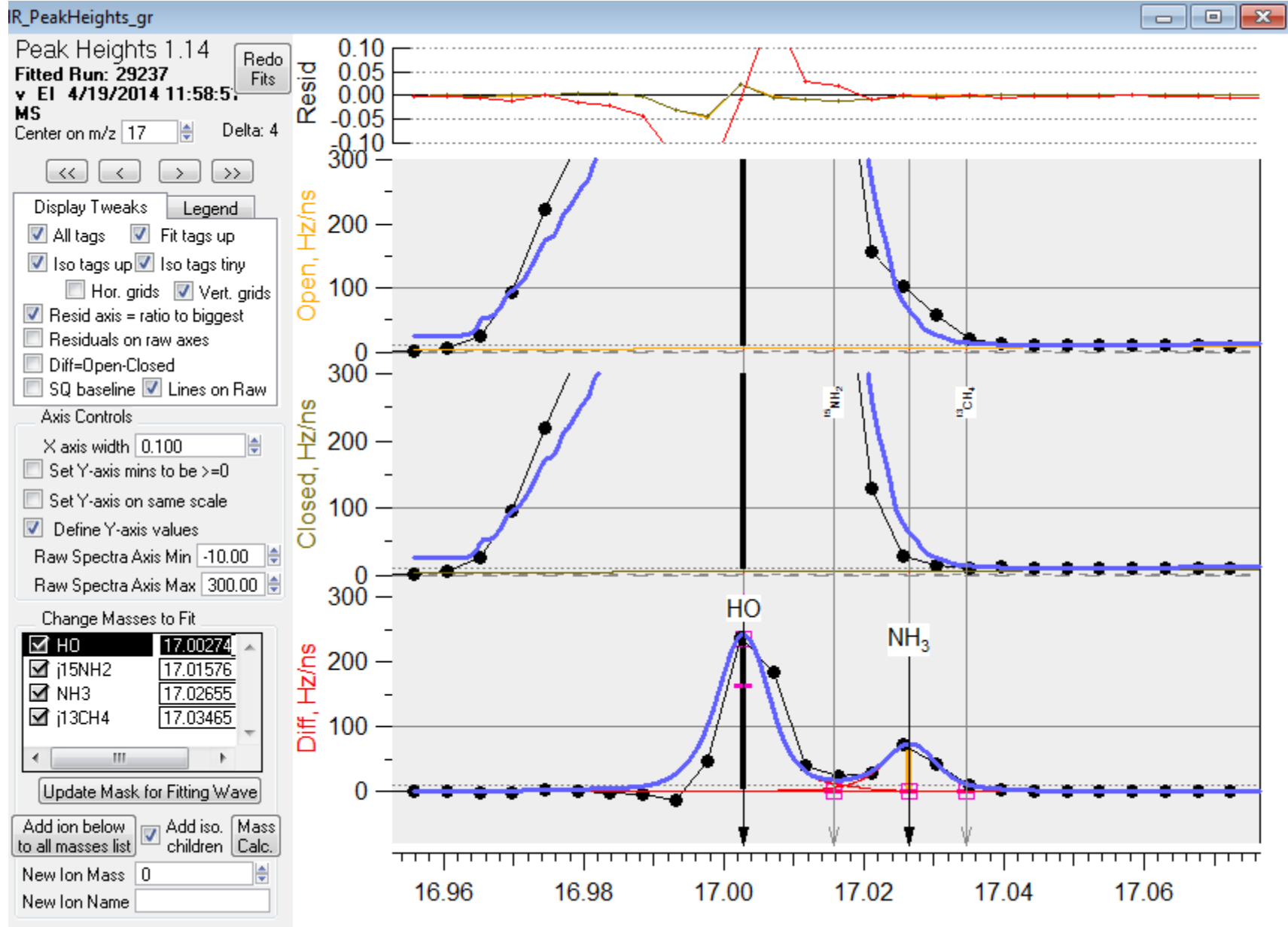
## Plot of OMinusC sticks and Diff sticks for NH, NH2, NH3, species HRNH4



NH and NH2 timeseries are identical. In this data set **NH3 was off by a ~ factor of 10 between OMinusC and Diff sticks!** Since NH3 contributes ~half of HRNH4, HRNH4 can be off by 50%.

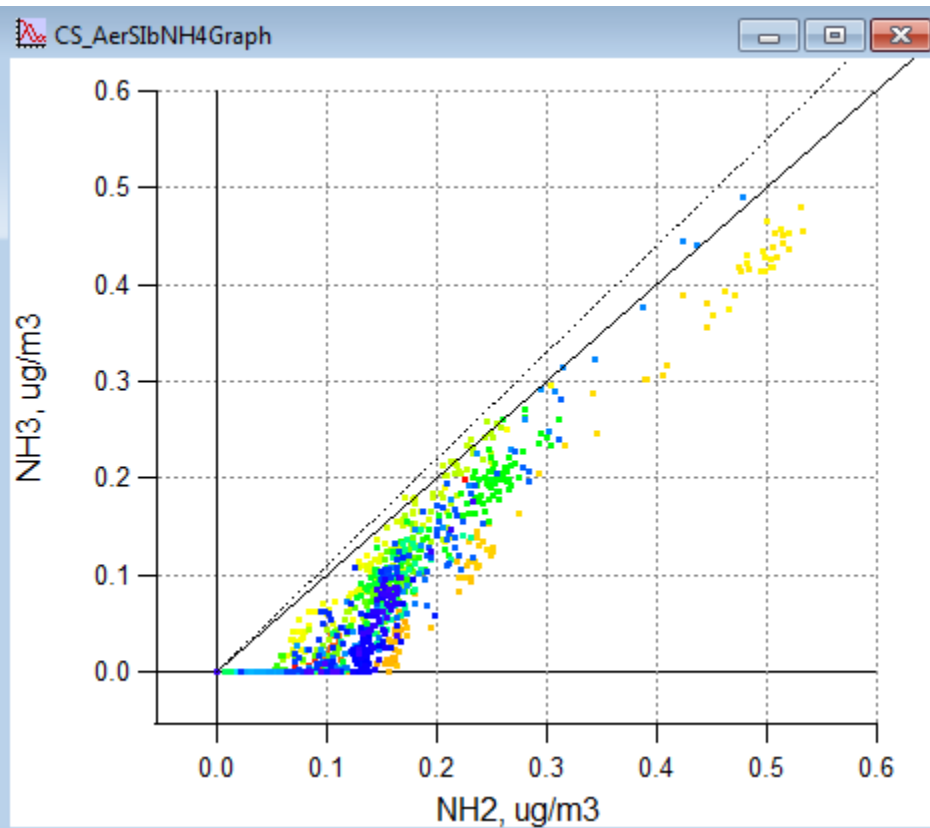
# NH3 Problem!!

Pika Plot at m/z 17. Same as slide 3. All y axis are the same scale.

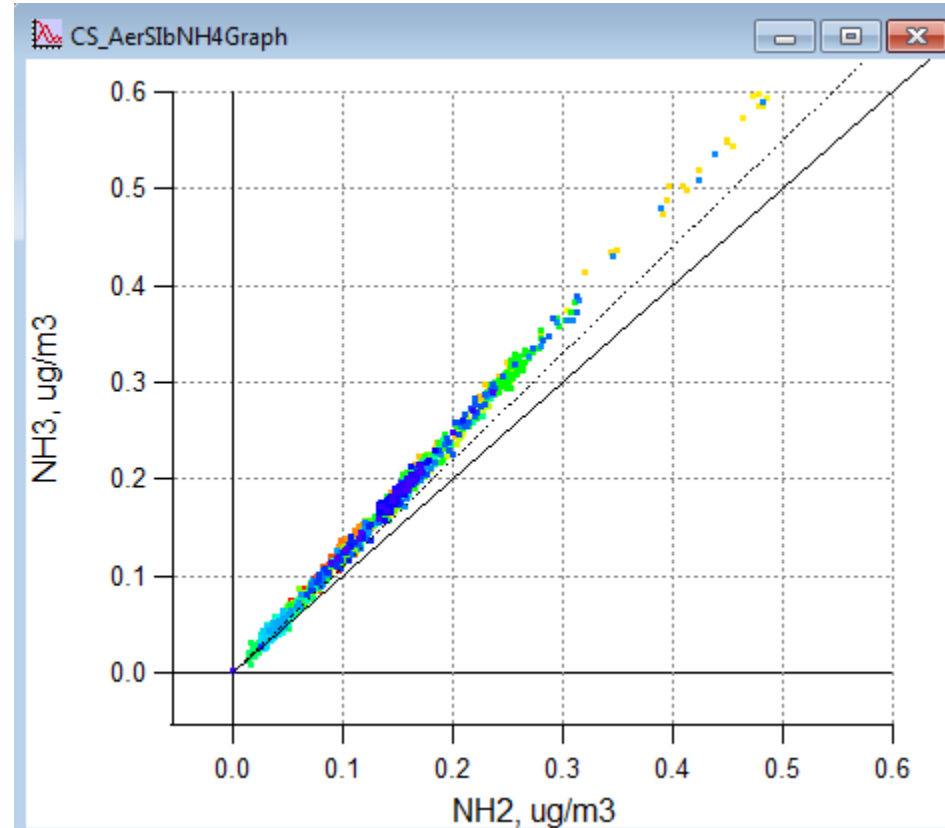


NH3 not fit well in Open and Closed... OMinusC data set for NH4 is 'bad'!

## NH3 vs NH2 OMinusC

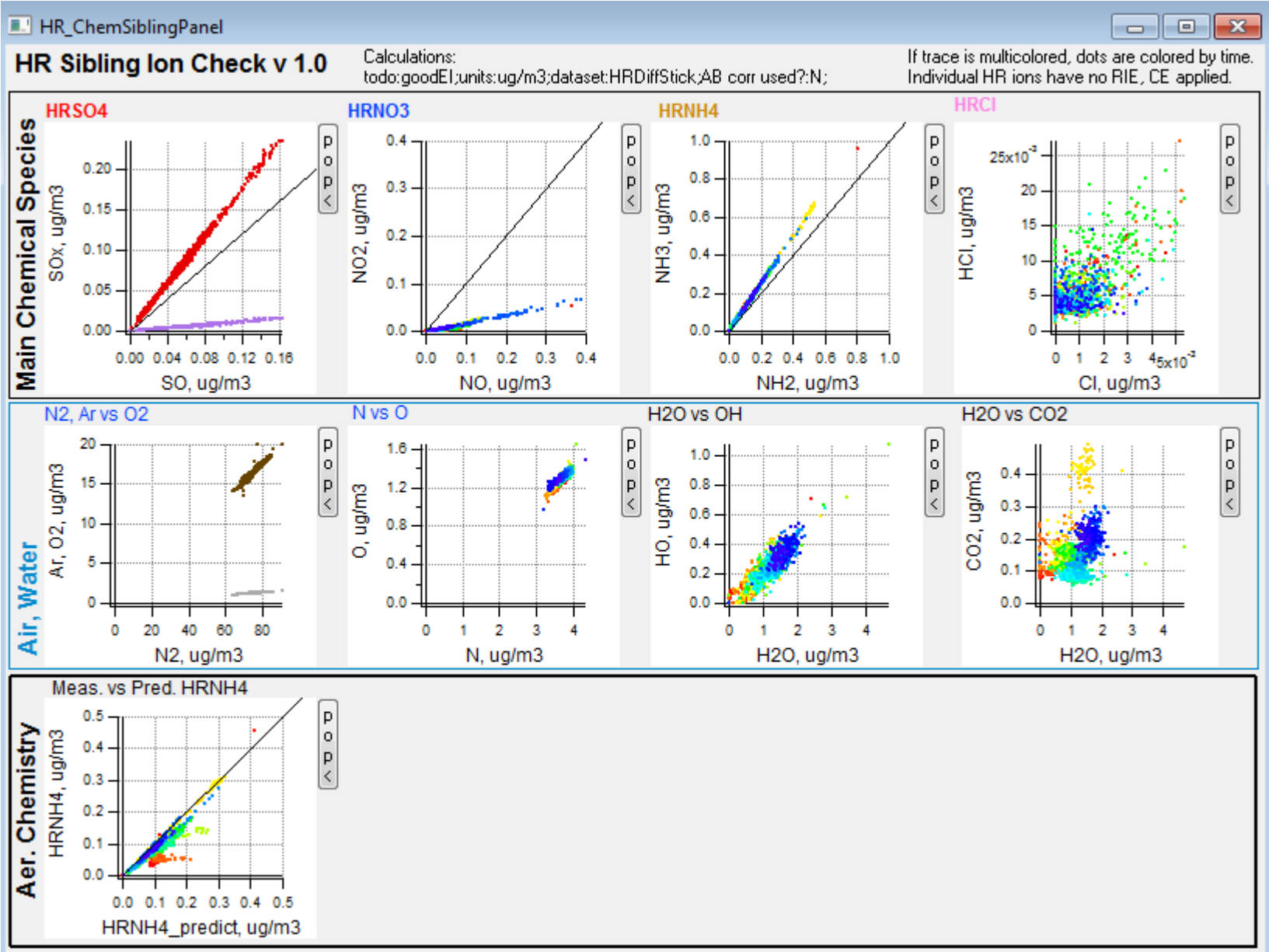


## NH3 vs NH2 Diff



Although nicely correlated in OMinusC, they should show a tighter correlation.

**Solution: Use HRDiff data set for HRNH4 species, or calculate NH3 as linear multiple of NH2.**



# HR Sibling Ion Diagnostic

HR\_Analysis\_Panel

## ToF-AMS HR Analysis 1.15P

PIKA module for SQUIRREL 1.56 or higher

Todo waves:

Version Website  
FAQs, Website  
Upgrade Pika  
Credits

Set Up HR Fits | HR Ion Groups | HR Fits One Spectra | HR Fits for Many Runs | **HR Results**

**Step 6i: Describe characteristics of HR results you want to generate.**

List of entities to generate

HR ions, families, and/or species (i.e. j15N,familyNH,HRair)   
\* The RIE and CE for HR ions and HR families is 1 (Nitrate Equiv.  $\mu\text{g}/\text{m}^3$ ).

Integer m/z   family

Data, Output Options

Data  Graph   Convert to  $\mu\text{g}/\text{m}^3$   Convert nan sticks to 0  
 Use MS AB correction  Convert neg. sticks to 0  
 Calc, plot err.   Set wave name suffix ^PTof data is dMdlq10dva

**Step 6ii: Select the time series or average mass spectra type of result to generate.**

Diag. | **Time Series** | Average MS | Elem. Anal. | 2-d Time Series MS | Export

Sq vs Pk Species

Useful Tables for Current Todo

Chemical Sibling Analysis (major HR ions in the same family)



# Care is still needed at dominate ions (air, water)

m/z	Dominate HR ion	Affected HR ions	Comments
28	N <sub>2</sub>	CO, C <sub>2</sub> H <sub>4</sub>	Important; CO is handled via HR frag table; C <sub>2</sub> H <sub>4</sub> can be important for elem. ratios
32	O <sub>2</sub>	S	Rarely important
18	H <sub>2</sub> O	NH <sub>4</sub>	Rarely important
17	HO	NH <sub>3</sub>	Important at high H <sub>2</sub> O
40	Ar	C <sub>3</sub> H <sub>4</sub>	Can be important for elem. ratios
44	CO <sub>2</sub>	CO <sub>2</sub>	Apportionment of aerosol & gas phase is handled via HR frag table
29	j15NN	CHO	Isotopic ratio less variable with ADQ card, CHO is handled via new HR Org Check Panel
39	K	C <sub>3</sub> H <sub>3</sub>	Dependent on surface ionization & tuning; Care needed for including K in BBOA; C <sub>3</sub> H <sub>3</sub> can be important for elem. ratios