1) Adding new ions into PIKA to account for marine organic aerosol ion fragments

2) Precautions for deciding when N containing ions peaks in fits are real or not

4th HR-AMS Clinic, Boulder, CO

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1) Adding new ions into PIKA to account for marine organic aerosol ion fragments
HR-ToF data collected (V mode) in marine environment

NaCl (m/z 58)
Diff ~ 90 Hz
Broad shape due to surface vaporization

…..and its isotope
(Na$^{37}$Cl, 1/3 of intensity of parent ion)
Found several “unknown” peaks in the MS

Likely halide clusters (Cl, Br) containing metals because they are on the left side of the m/z (also in closed, surface vaporization)

Like this at m/z 125 (MnCl$_2$)
How do I make sure my guessed mass is right?

Use the isotope ratios of Cl, Br etc.…. If MnCl$_2$ is real, there should be

1) MnCl$^{37}$Cl at mz 127 (UMR value)

2) Mn$^{37}$ClCl at mz 129 (UMR value)
Need to modify the HR ion lists

Still some unknowns....
Use mmass.exe (public software)
...once you fitted all the peaks (and properly modified HR batch, family and frag tables)
2) Precautions for deciding when N containing ions peaks in fits are real or not

Average todo wave w/ C3H2N
No C3H2N….there seems to be a residual signal to be fitted

One run….no clear sign that C3H2N should be fitted
Look at Ar (m/z 40)

Look at SO (m/z 48)
Bottom line

- N containing peaks are small, and they usually fall in the tail of big signals. The “peak broadening” can be an issue here

- Look at average todo wave vs single run

- Evaluate peak shape using Ar and SO

- Look at time series and their noise
- Look at correlation plots between main peak and small ion (eg C4H4 and C3H2N of slide 16) to see if they co-vary: if yes, the small ion is not real

- Look at average todo wave vs single run

- Use W mode if you have it 😊