Development of Event Trigger data analysis approach for single particle characterization

(Event trigger data from SP-AMS)

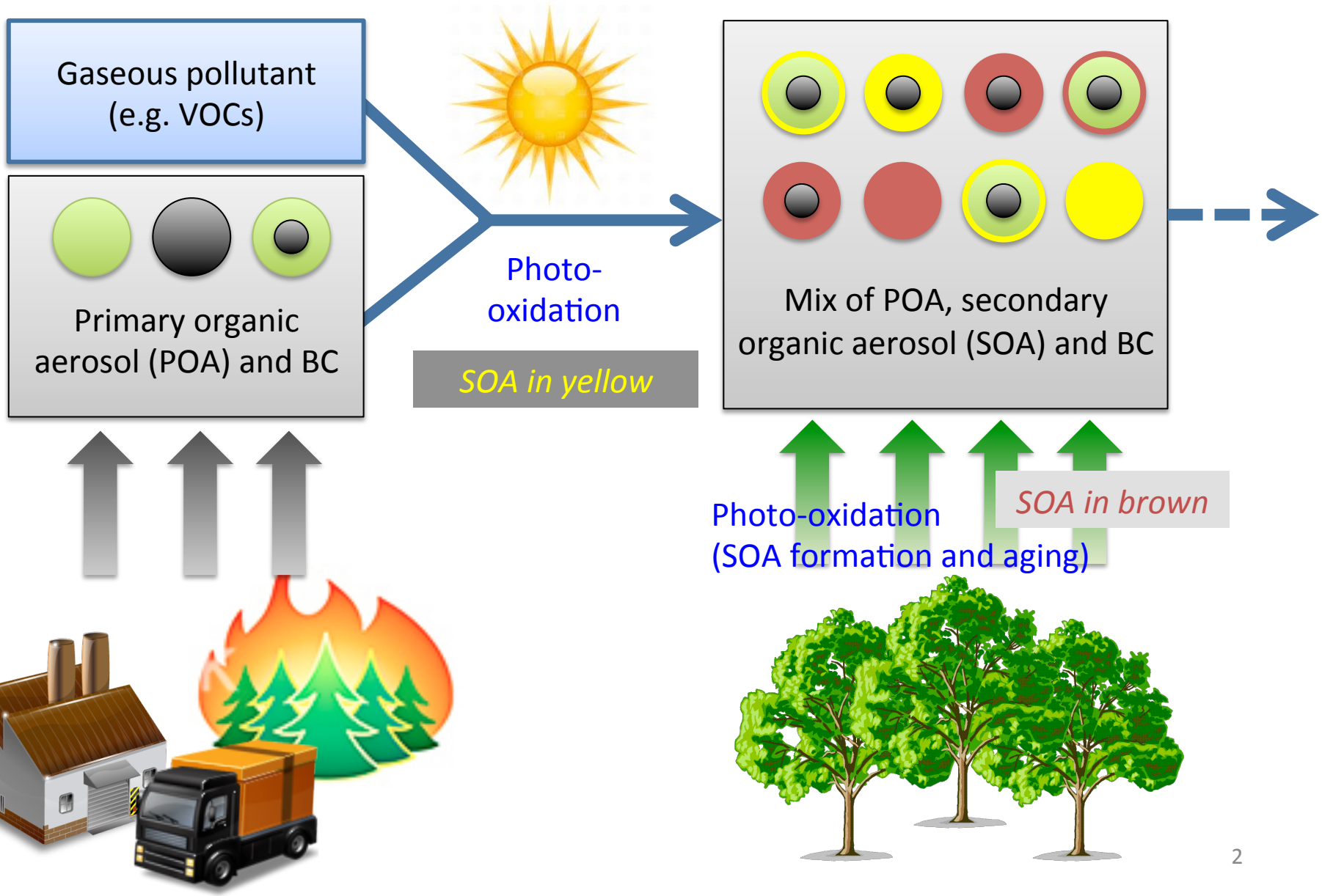
Alex K. Y. Lee[1], Megan Willis[2], Jonathan P.D. Abbatt[2]

[1]Department of Civil and Environmental Engineering, National University of Singapore

[2]Department of Chemistry, University of Toronto, Canada

17th AMS users meeting, Oct 23, 2016

Formation of organic coating on BC particles



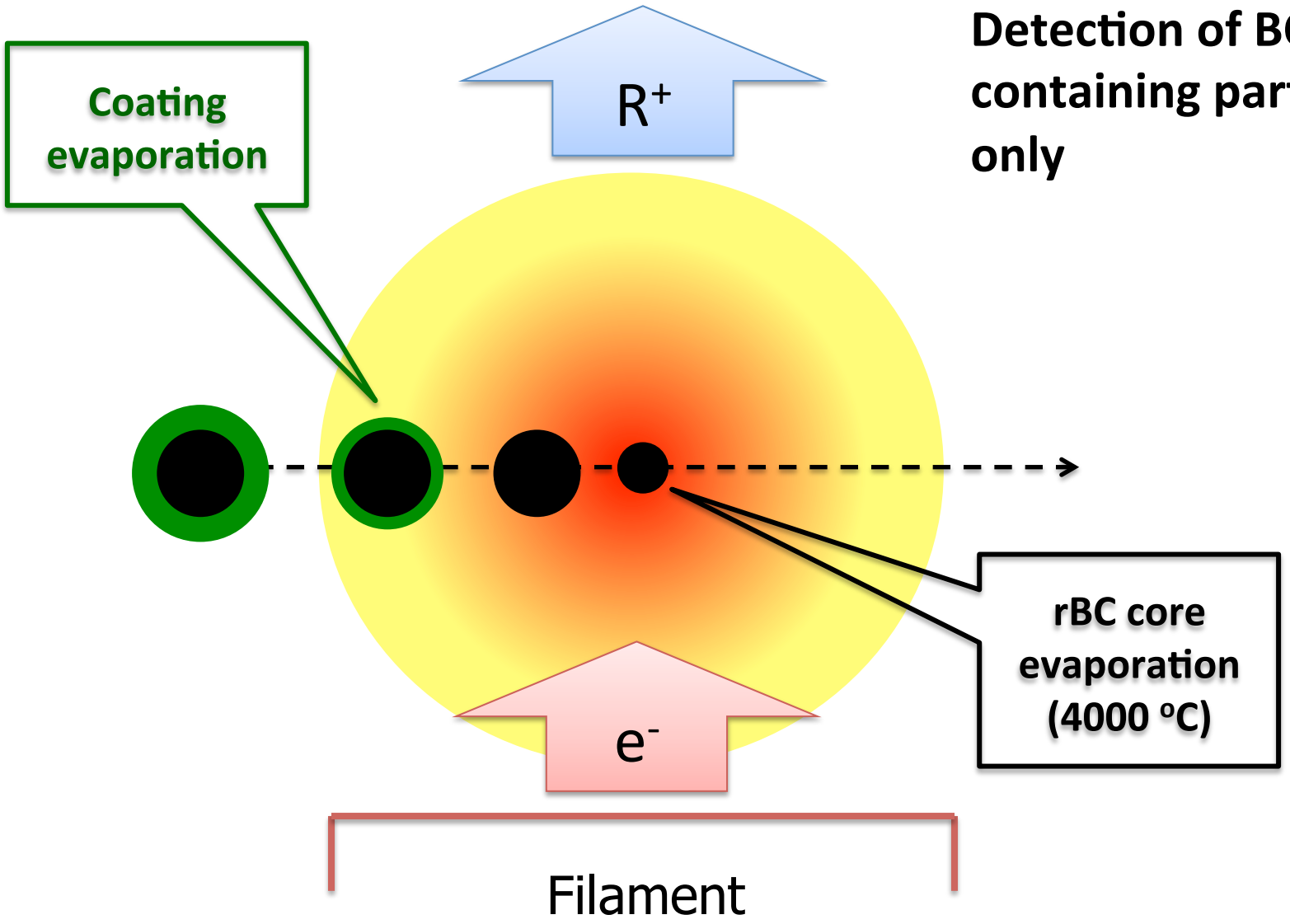
Sampling period and location – Fontana, CA

July 4-28, 2015

~ 80 km east of Los Angeles

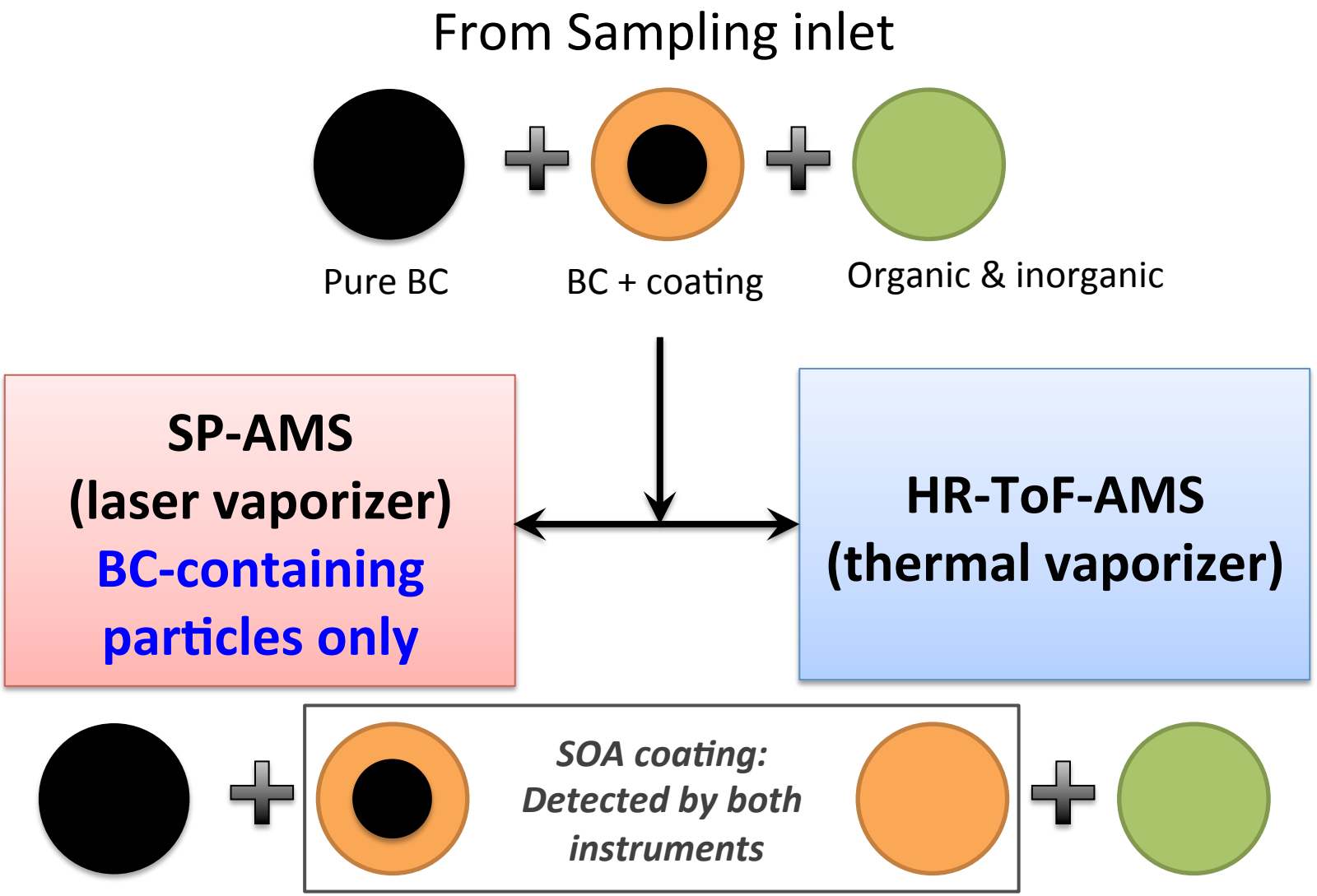
South Coast Air Quality Management District-managed site *(Fontana Fire Department at 14360 Arrow Highway)*

SP-AMS (Thermal vaporizer removed)



Onasch et al., 2012, Aerosol Sci. Techno., 46, 804

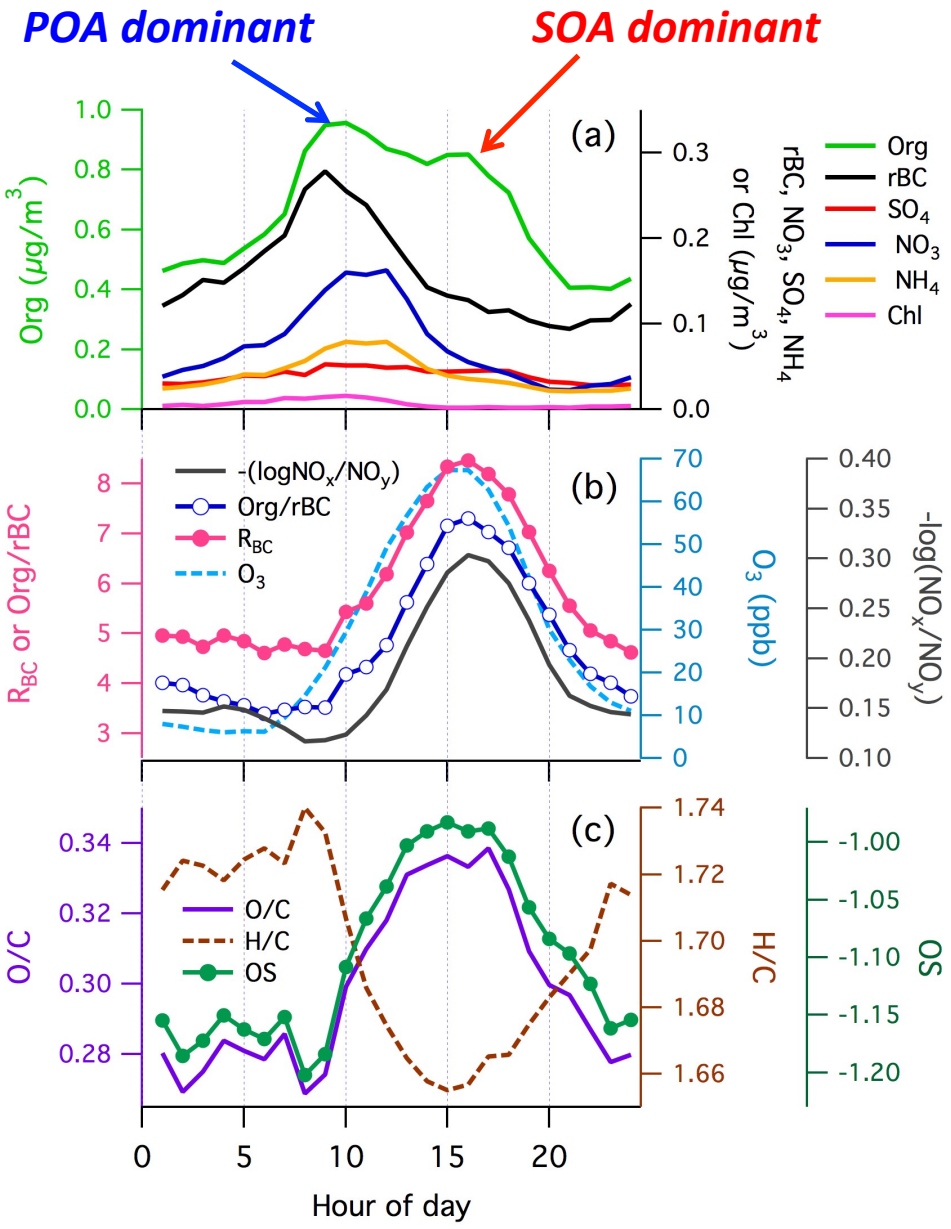
Soot particle aerosol mass spectrometer (SP-AMS) vs. HR-ToF-AMS



Formation of SOA coating on BC surface

Coating thickness

R_{BC} = NR-PM/rBC or Org/rBC

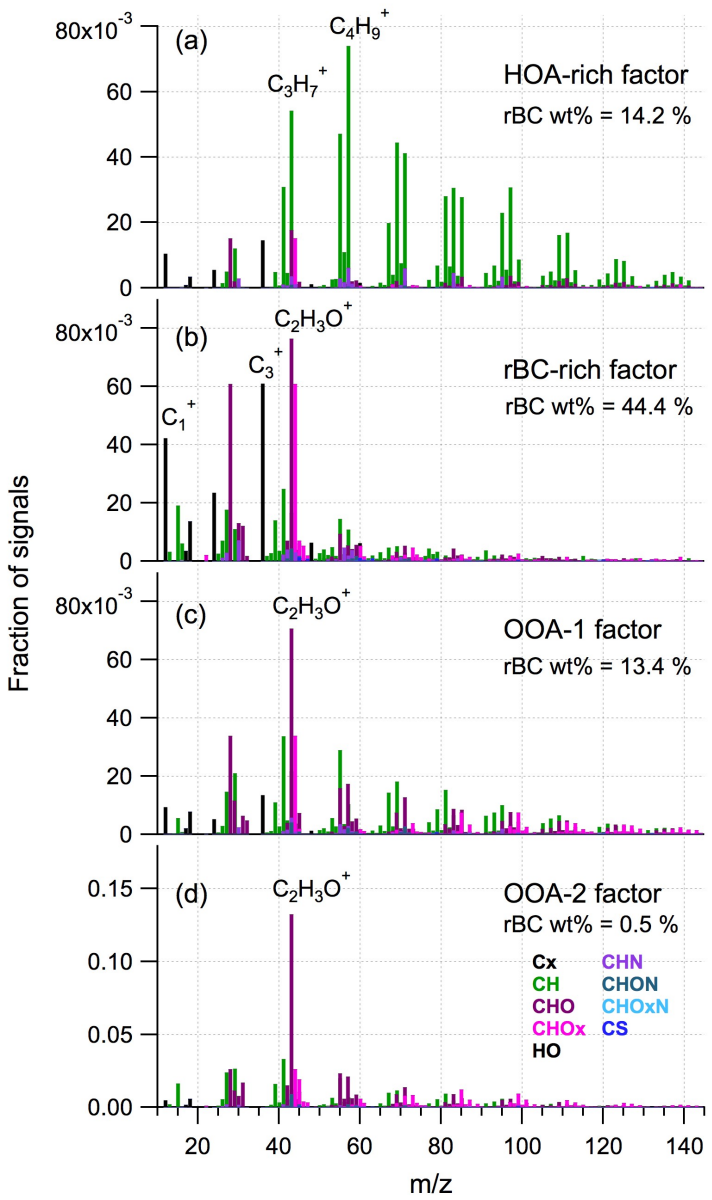


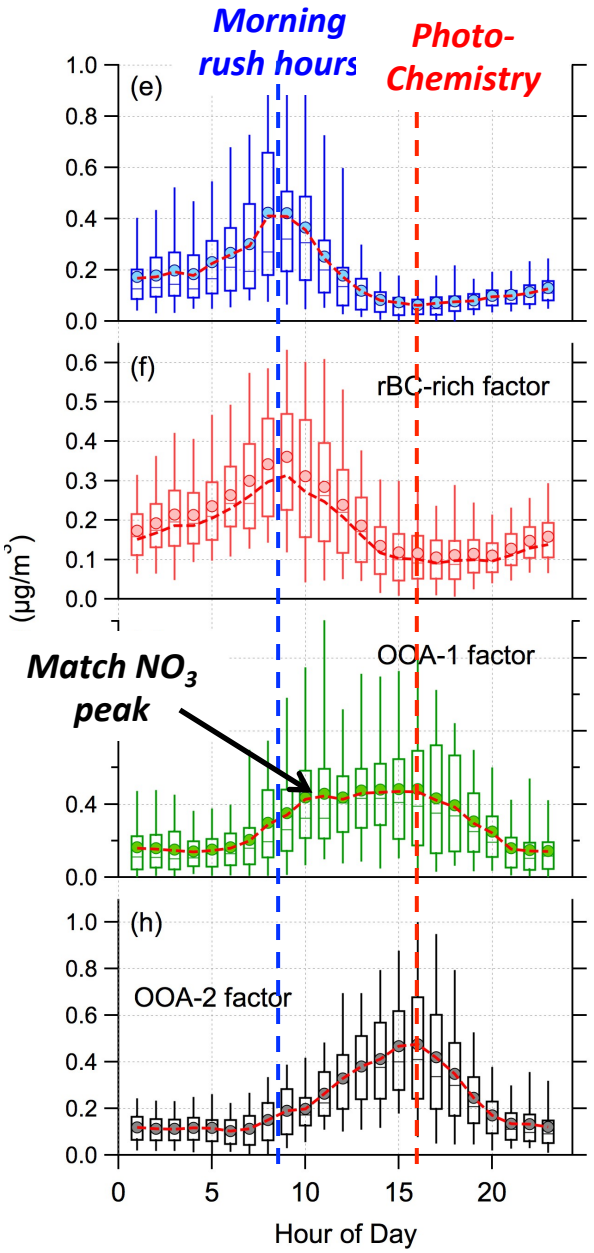
Photochemical clock

$-\log(NO_x/NO_y)$ α exposure time to [OH]

Higher O/C and oxidation state (OS) for SOA

PMF analysis: 4-factors solution



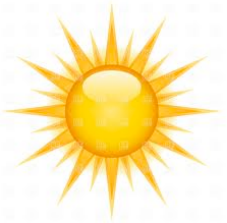


Hydrocarbon-like OA (HOA)-rich factor

rBC-rich factor

(with the support of single particle characterizations)

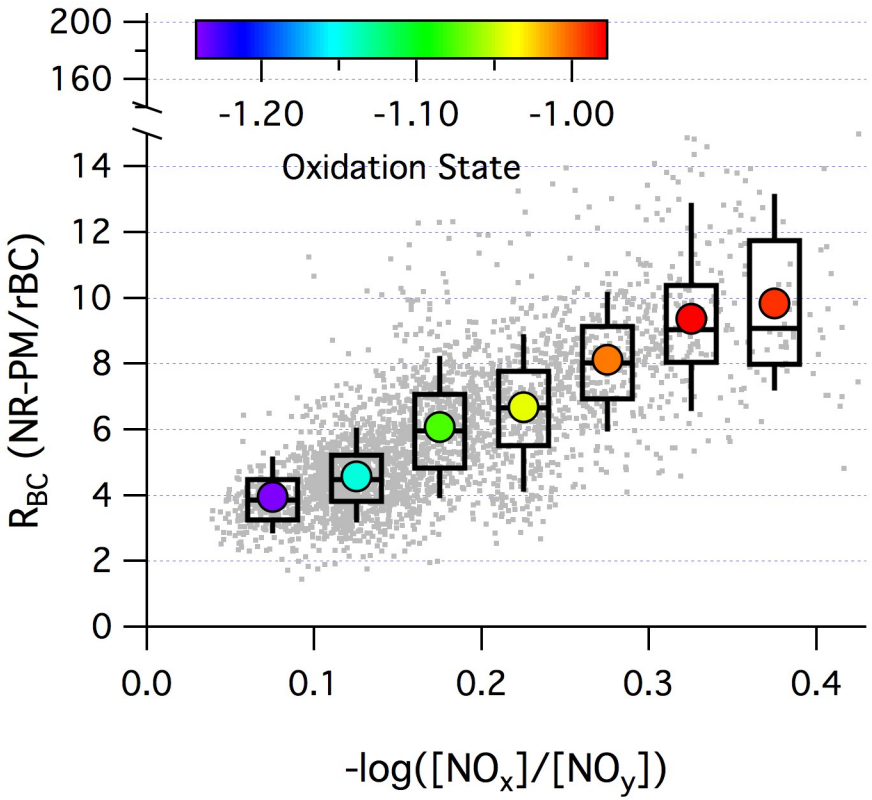
Oxygenated OA
OOA-1 factor

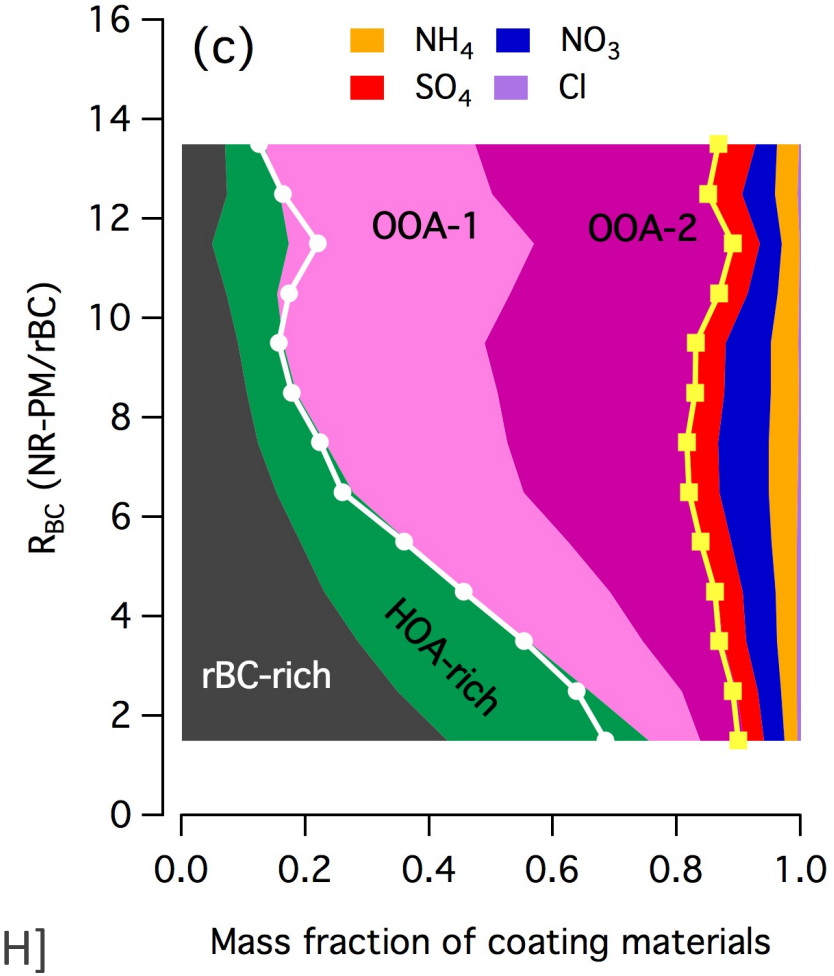


OOA-2 factor

Photochemical age: Fresh or aged SOA?

OOA-1 & OOA-2 → Fresh SOA





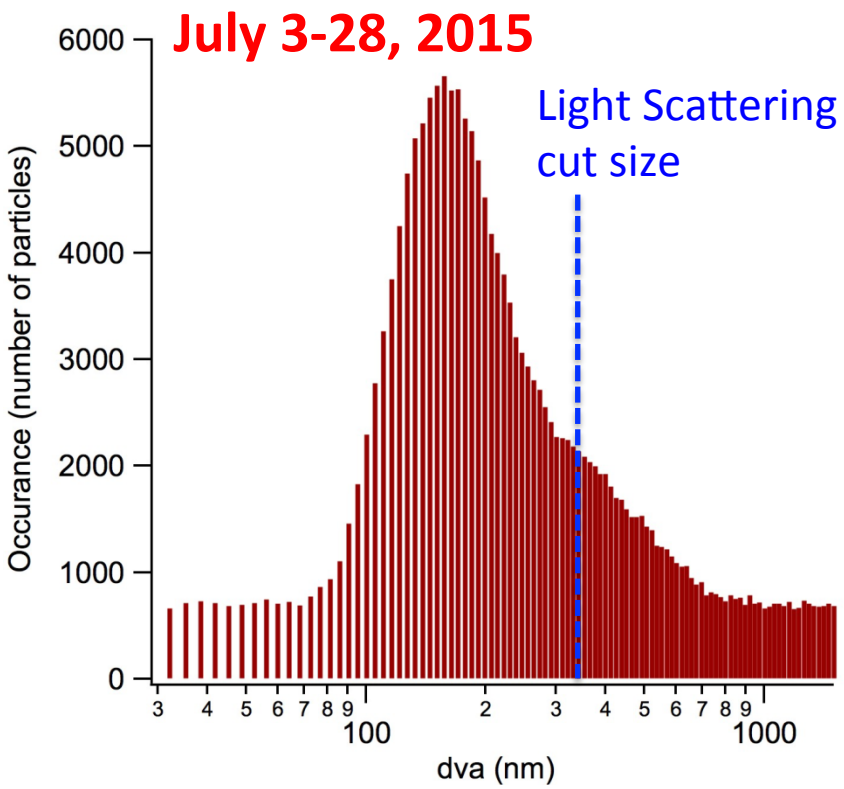
Photochemical age = -log([NO_x]/[NO_y])/k_{rxn}[OH]

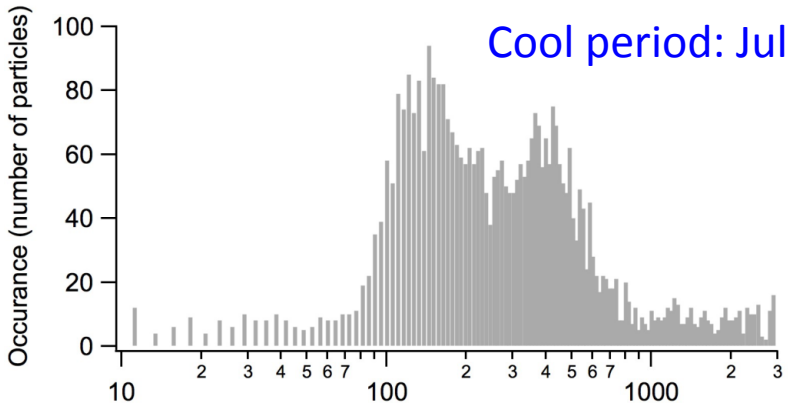
k_{rxn} = 7.9 x 10^{-12} cm^{-3} $molecules^{-1}$ s^{-1}, [OH] = 4 x 10^6 molecules cm^{-3}

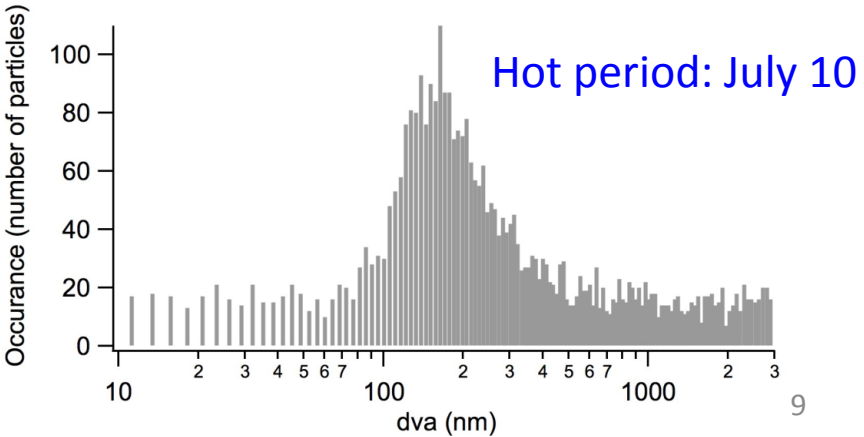
Single particle detection: Event trigger (ET)

SP-AMS menu setting (2 min per 10 min cycle)

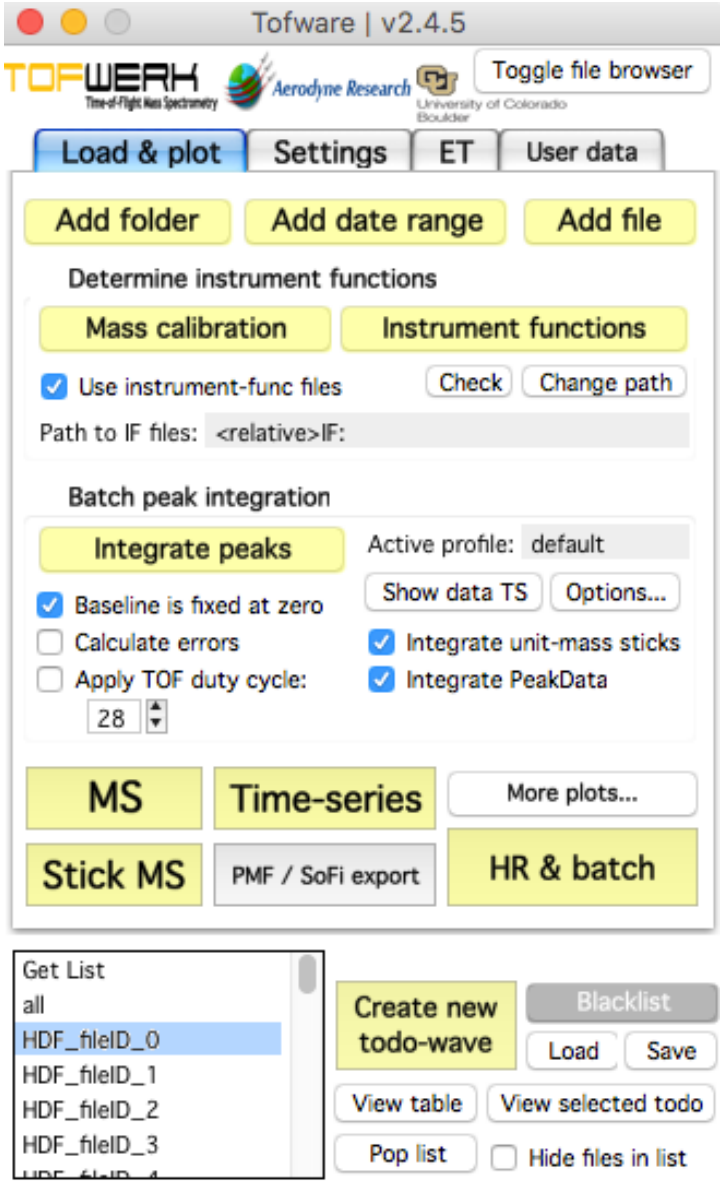
- ROI1: m/z 45-150 (Org) – 5 ions → **Nitrate, sulfate, organic**
- Or ROI2: m/z 43 (Org) – 4 ions → **Organic**
- Or ROI3: m/z 36 (BC) – 3 ions → **Black carbon**
- **Number of particles:** 410,100 (~10,000 using LS in Toronto)





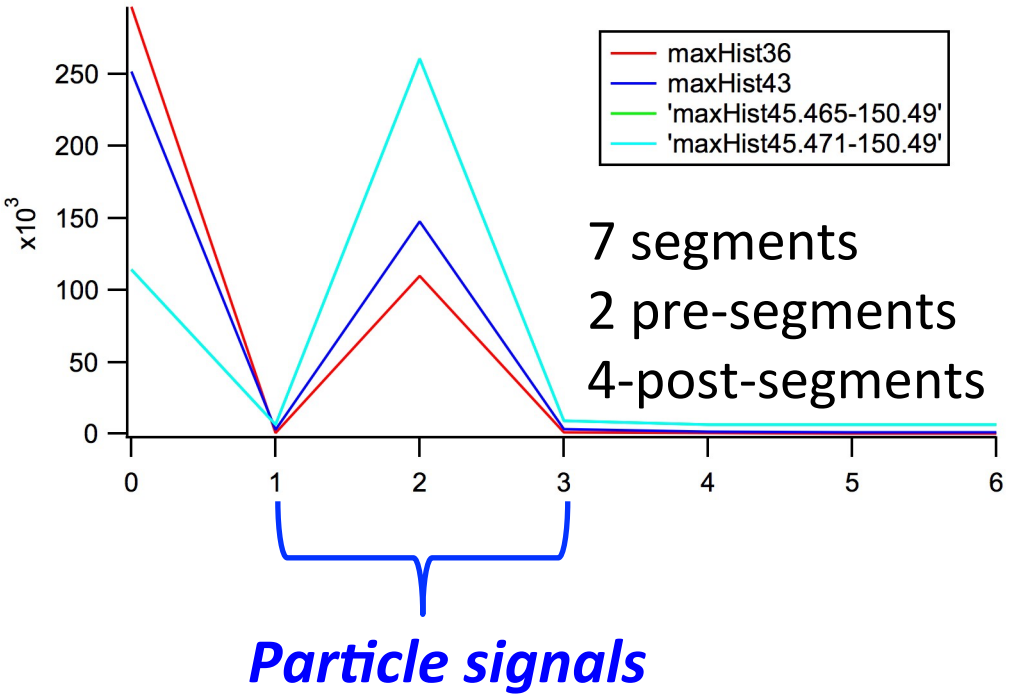


Tofware (v2.4.5) – Data pre-processing

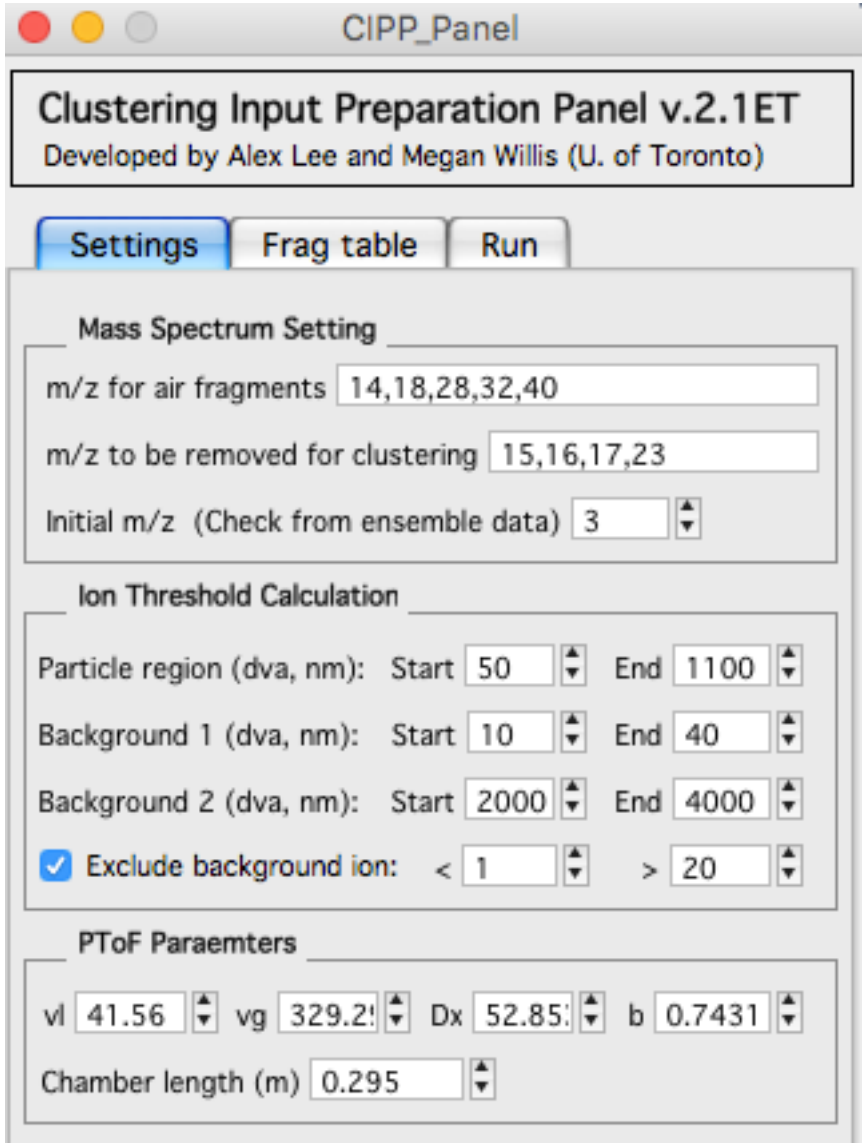


From Tofware:

- ChopTimes (pToF data)
- MSSft_all (MS matrix)
- t_start_wr (time)

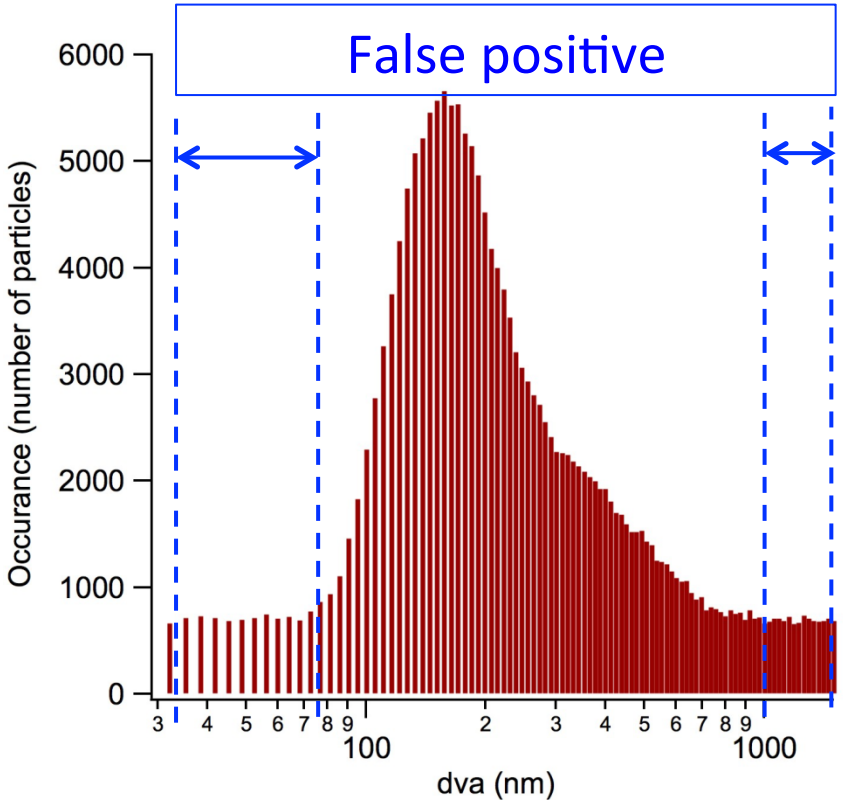


Clustering Input Preparation Panel (CIPP)

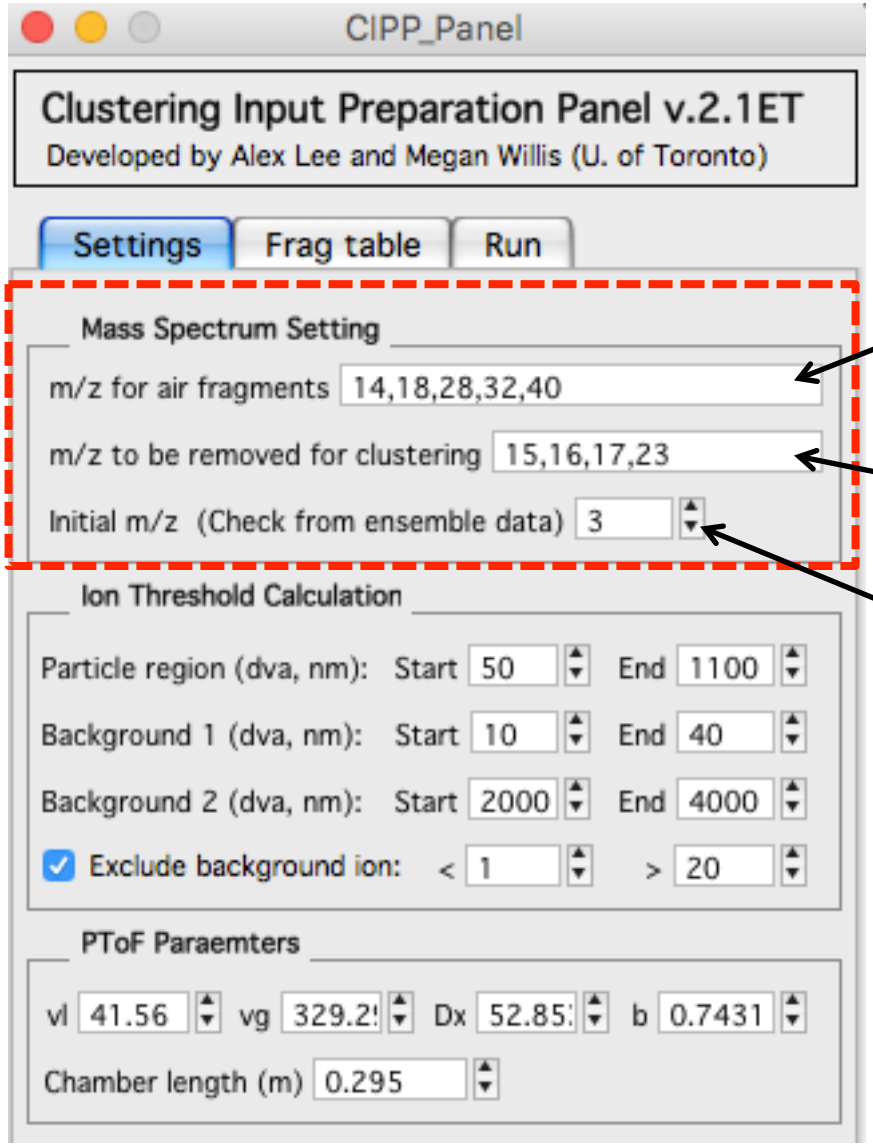


Main Functions:

1. Remove false positive (or identify real particles)
2. Prepare waves and matrix for cluster analysis



Remove false positive (or identify real particles)



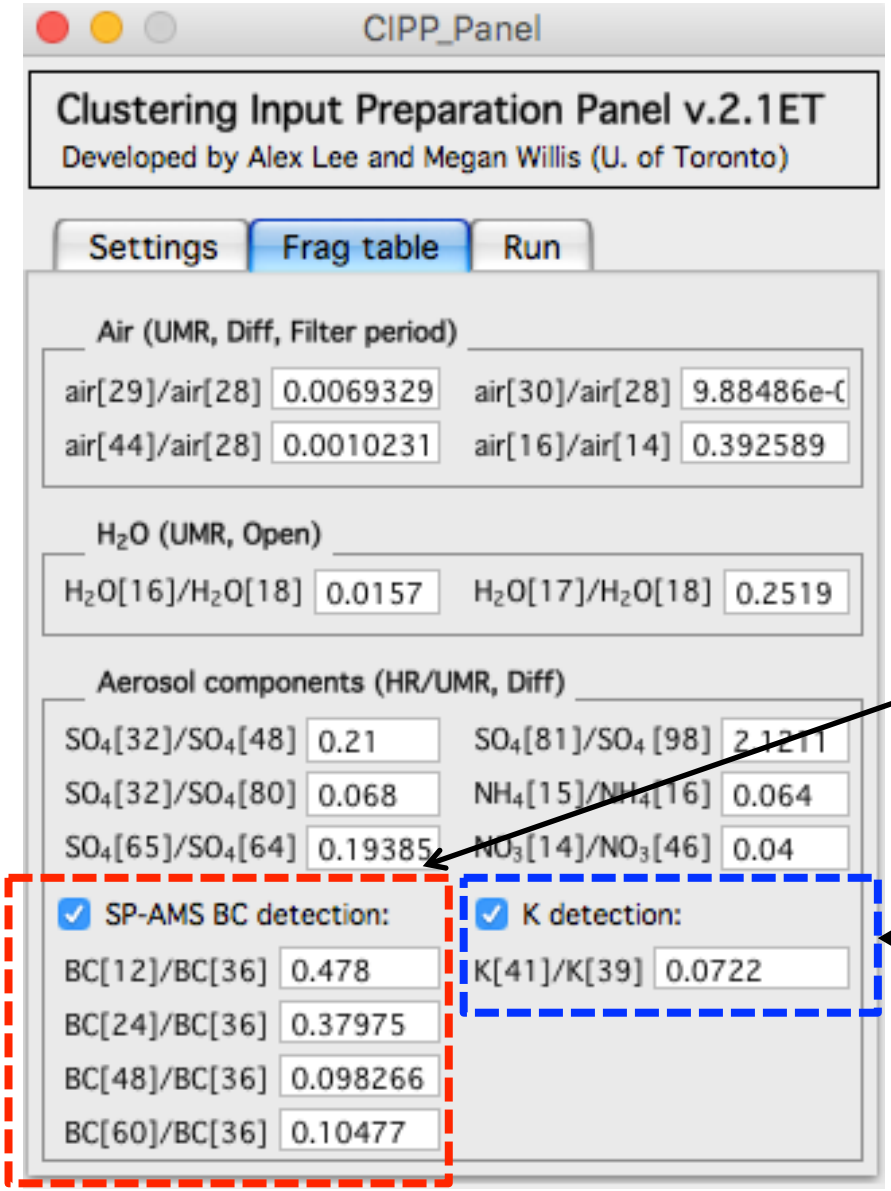
Step 1: Calculate total ion signals of individual event

Remove air fragment from the matrix for total ion calculation and cluster analysis

Remove m/z from the matrix for cluster analysis

The first m/z of MS

Remove false positive (or identify real particles)



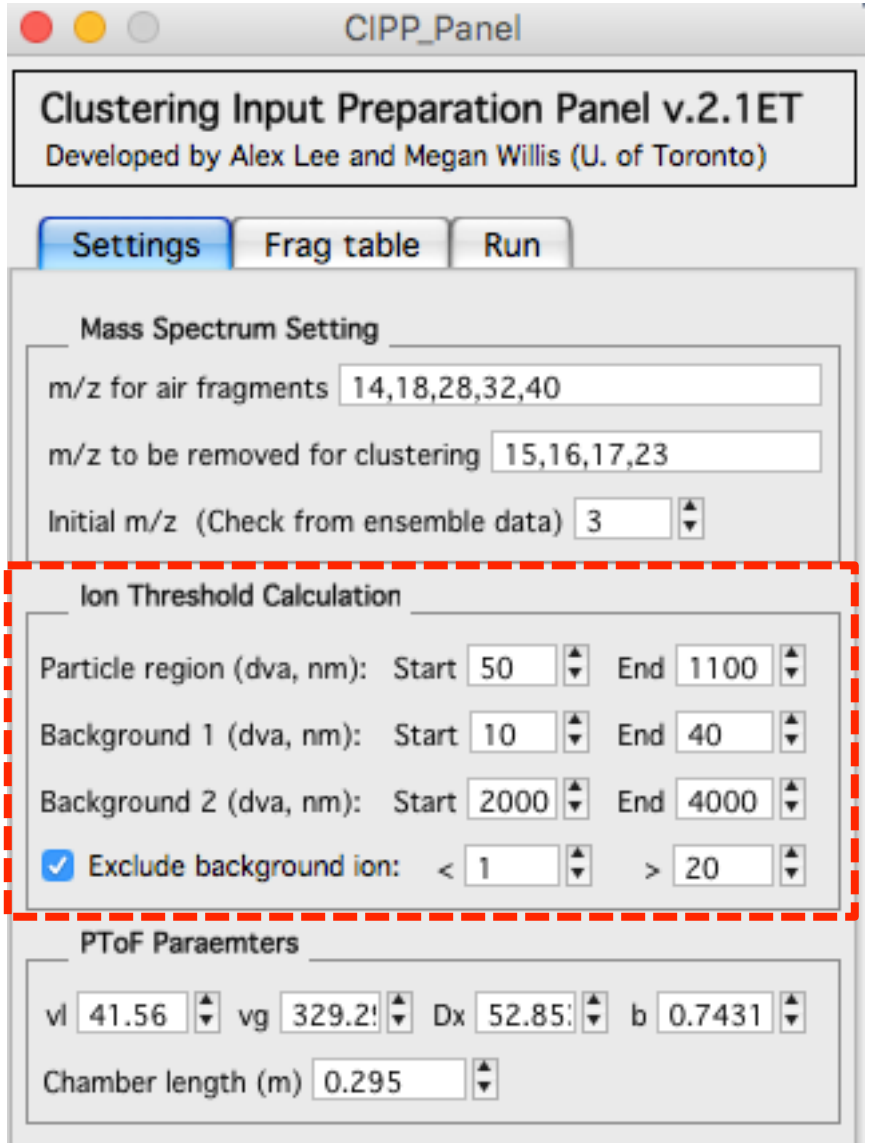
Simplified fragmentation table

- Parameters are determined from UMR and HR ensemble data or default fragmentation table in squirrel

"BC" option for SP-AMS data

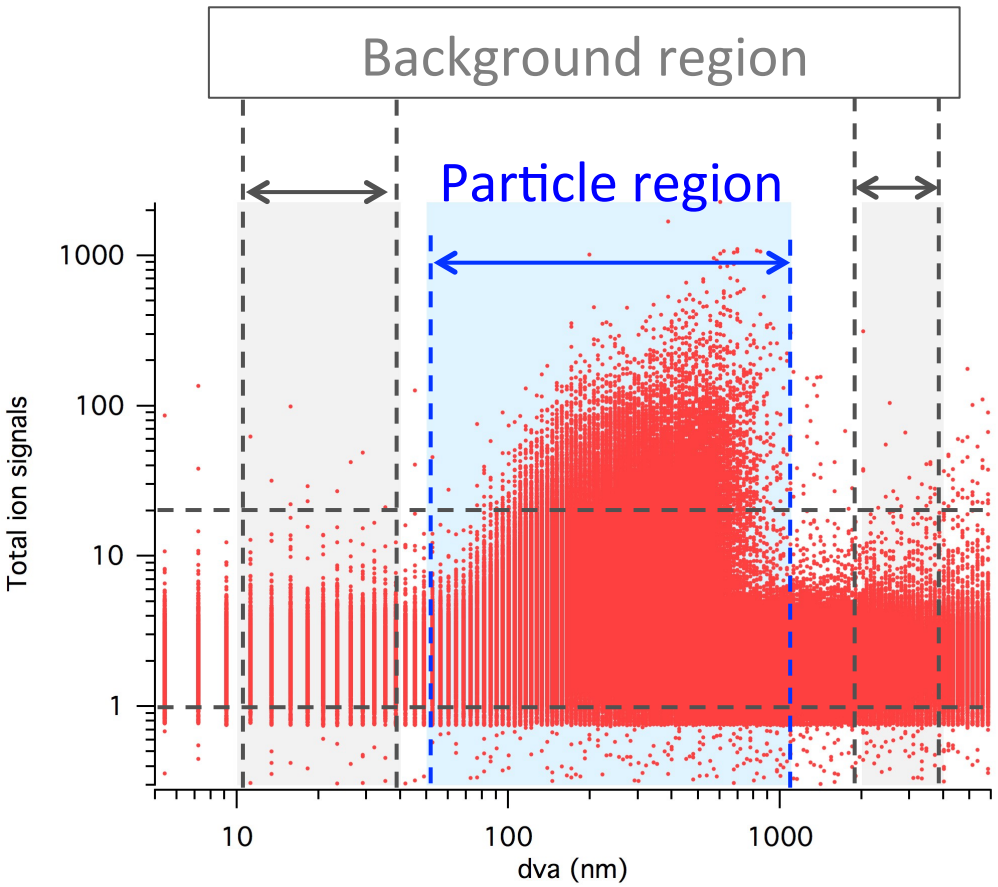
"K" option for data with strong BBOA signal

Remove false positive (or identify real particles)

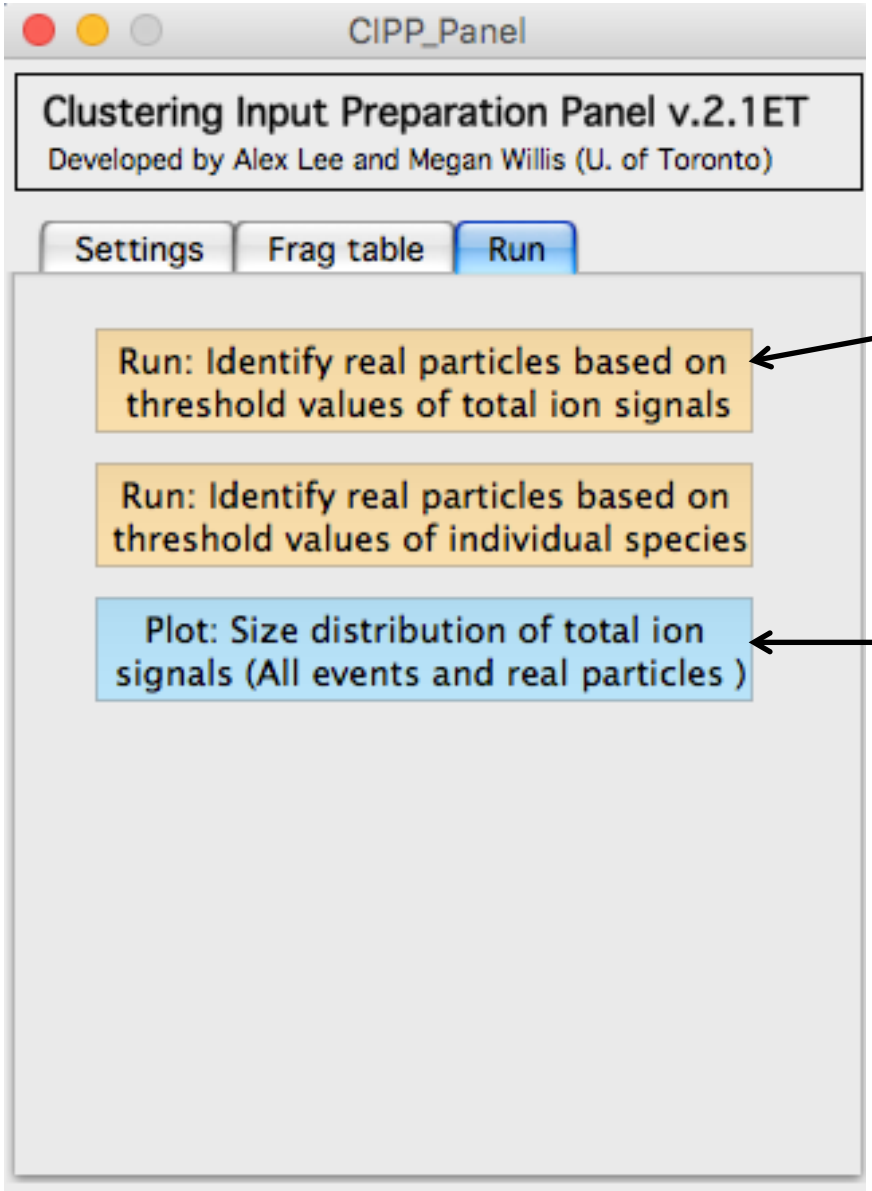


Step 2: Calculate ion threshold for real particle events

Threshold = Mean +3*std deviation



Clustering Input Preparation Panel



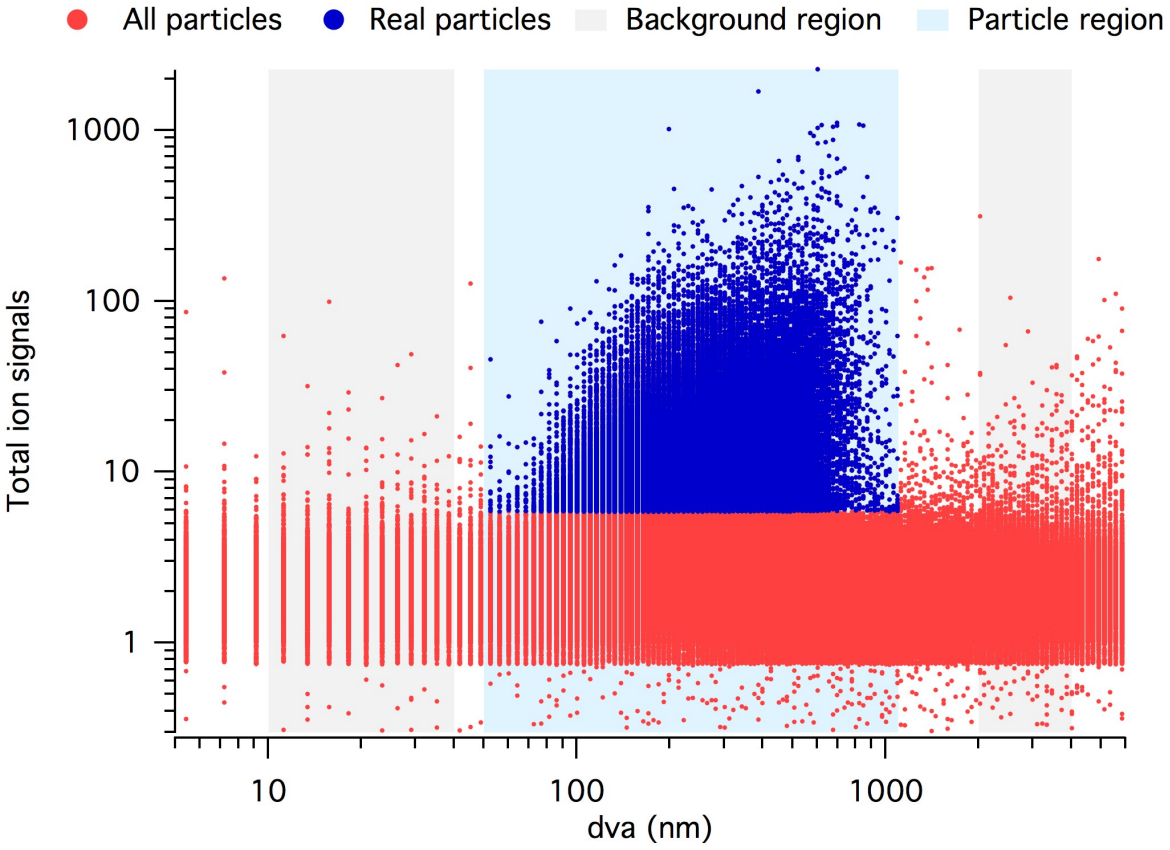
Run the ion threshold calculation (total ions)

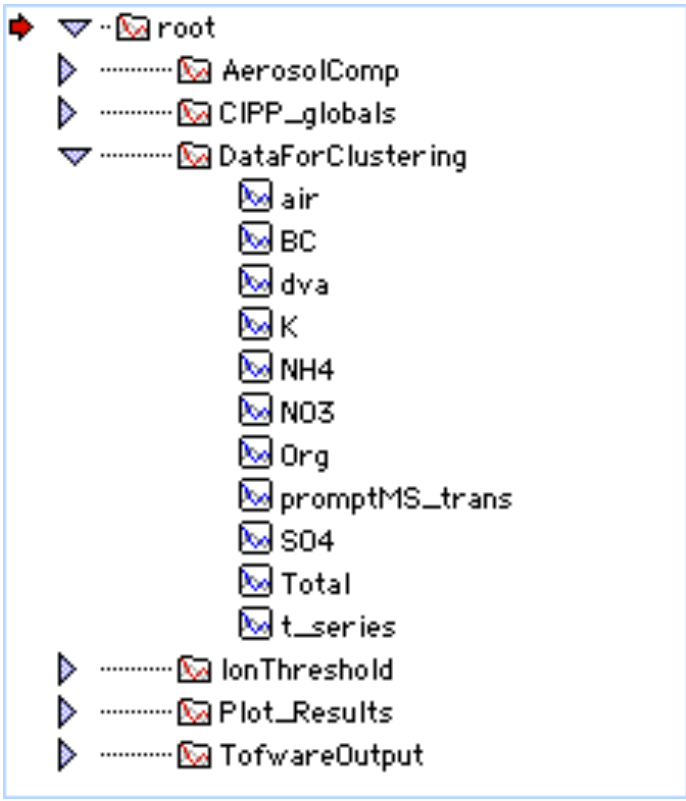
Plot the results

Results from CIPP

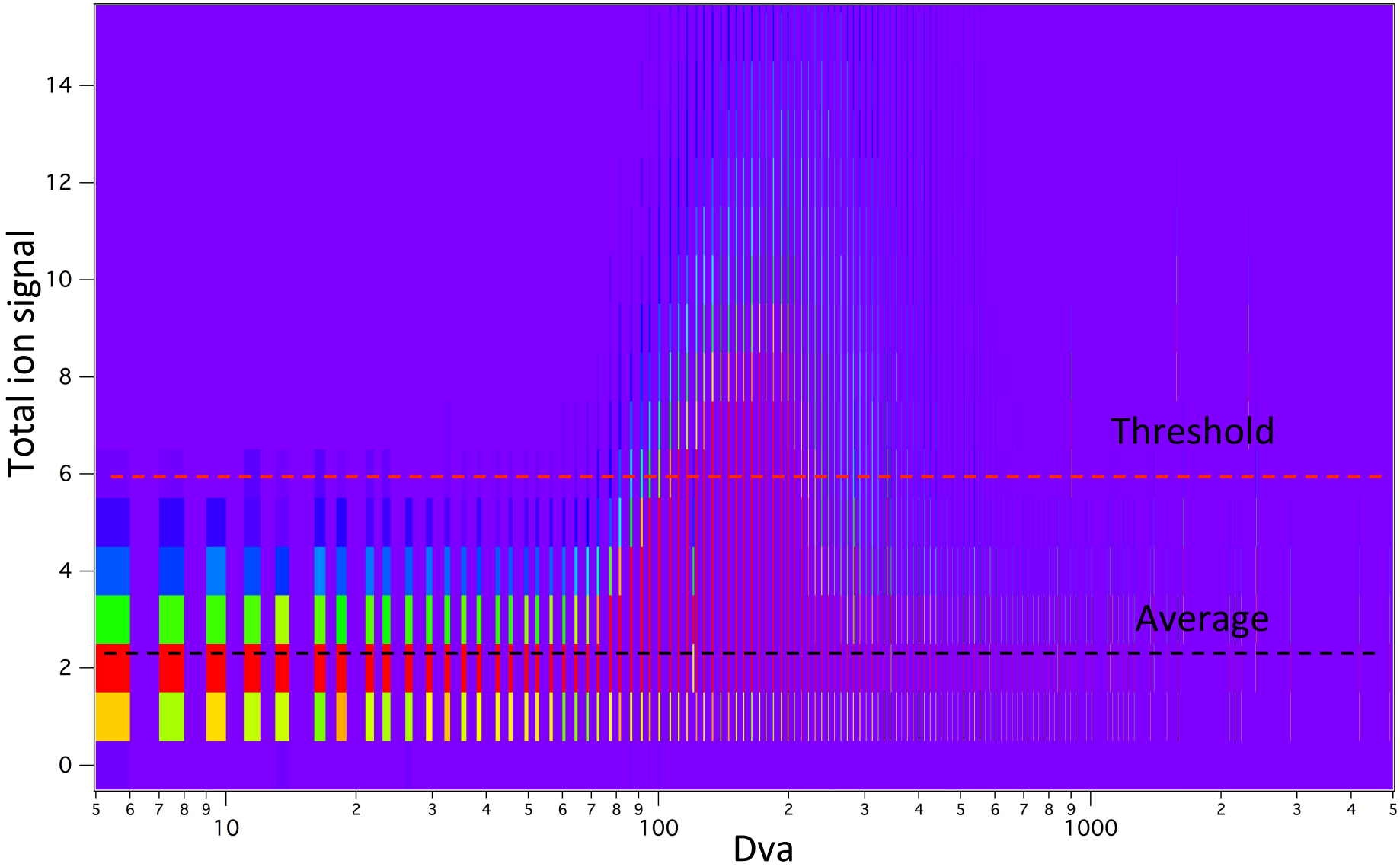
Background average = 2.2932
Total ion threshold = 5.8609

Standard derivation = 1.1892
Particle # = 70695 of 4.101e+05 (17.238%)

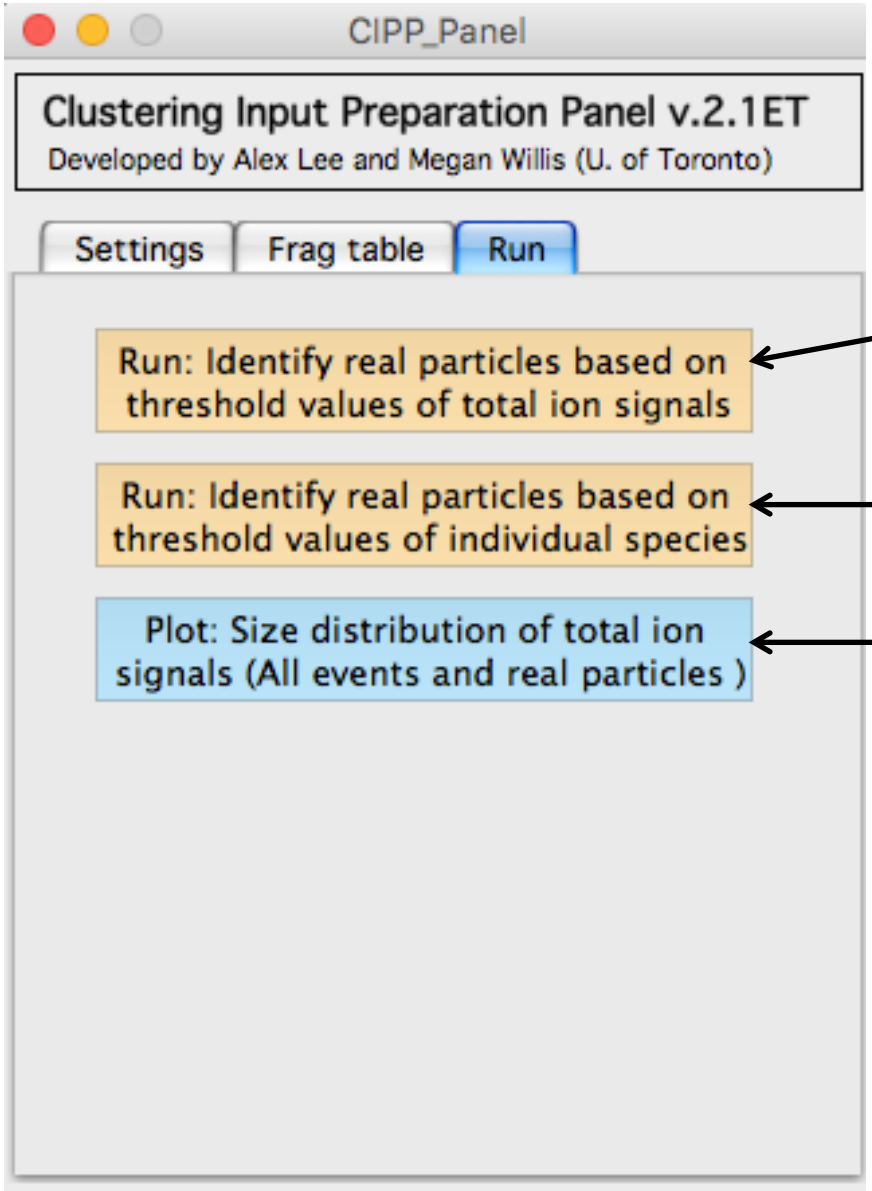




Setting the threshold too high?



Clustering Input Preparation Panel

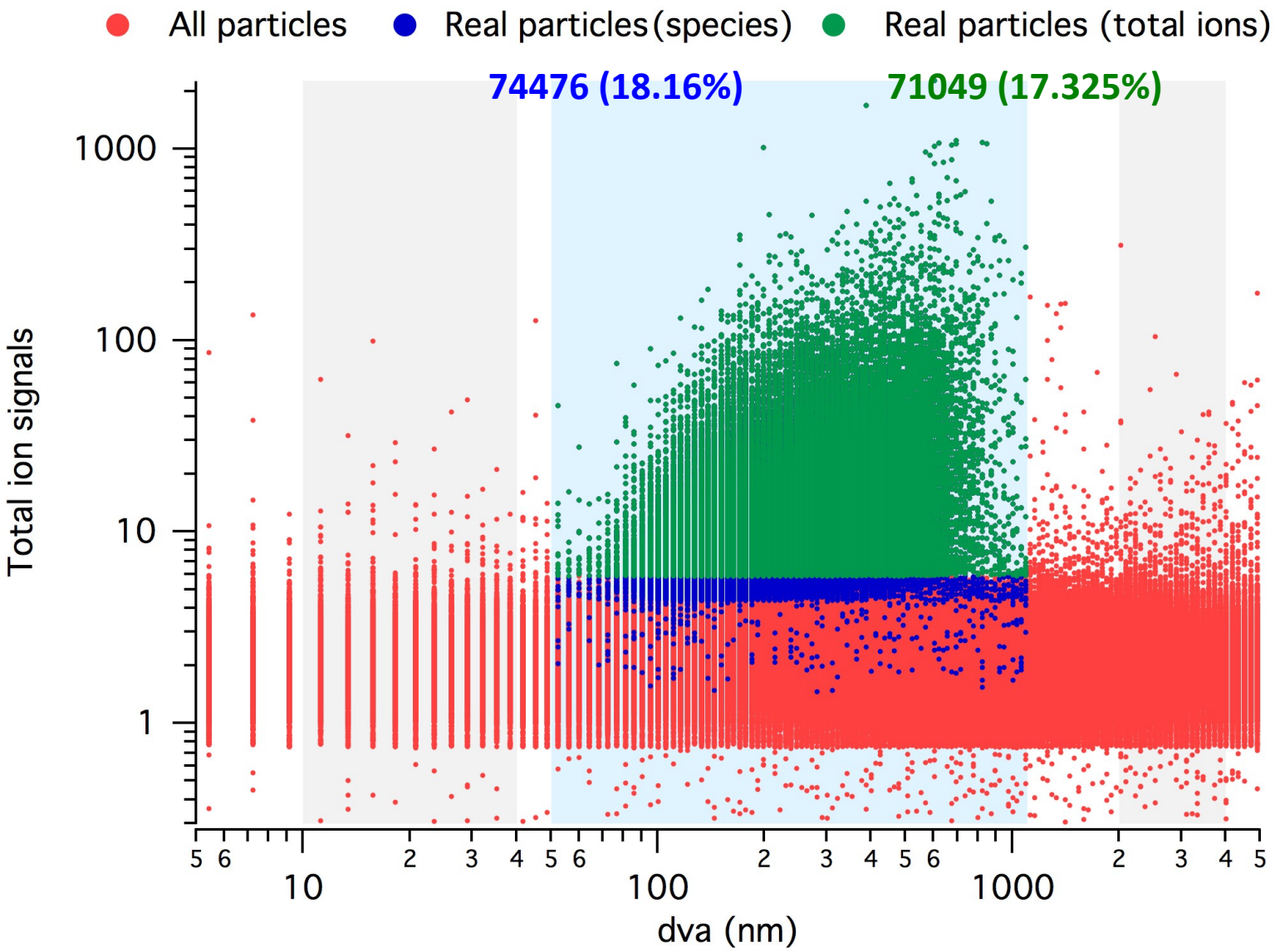


Run the ion threshold calculation (total ions)

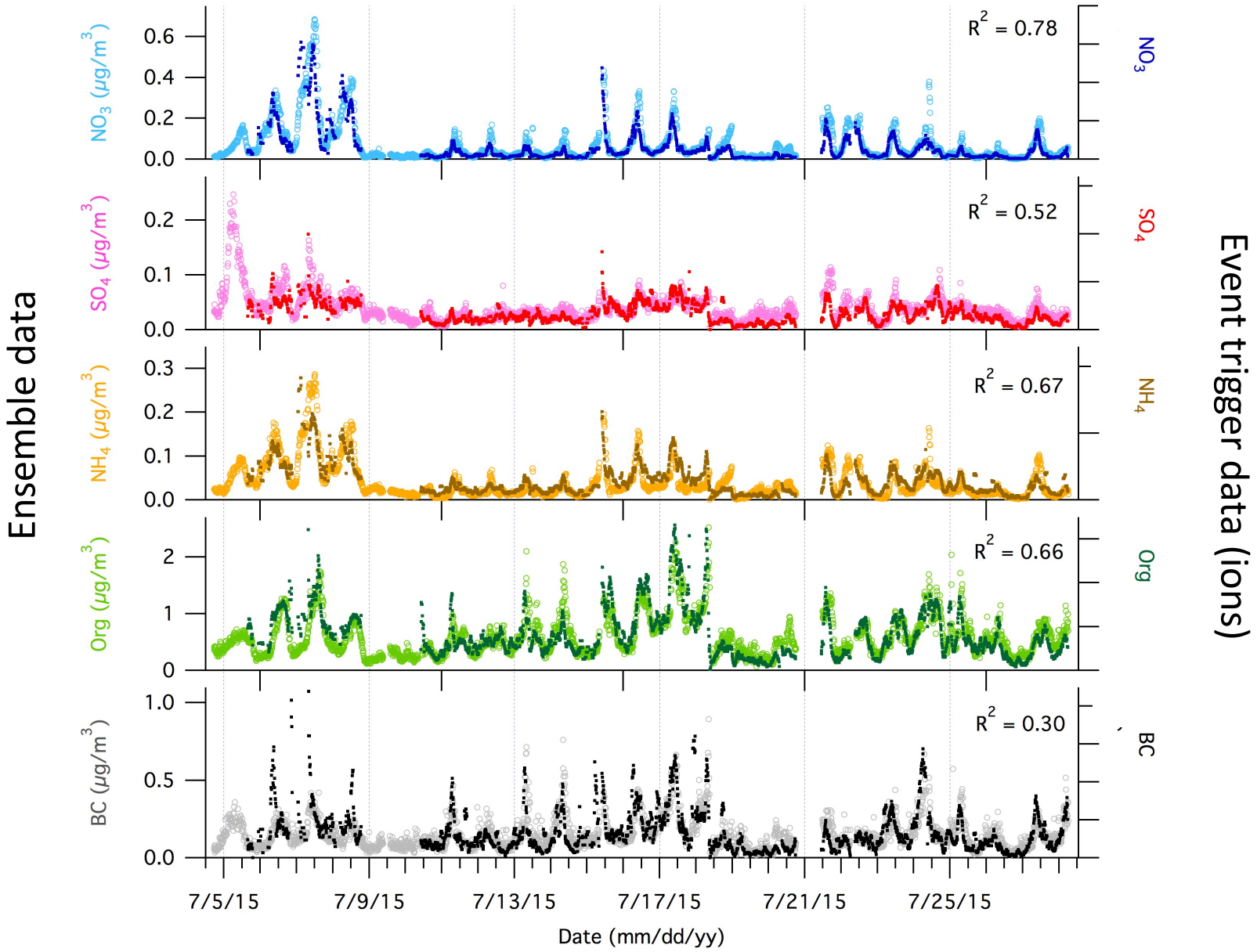
Run the ion threshold calculation (species, testing)

Plot the results

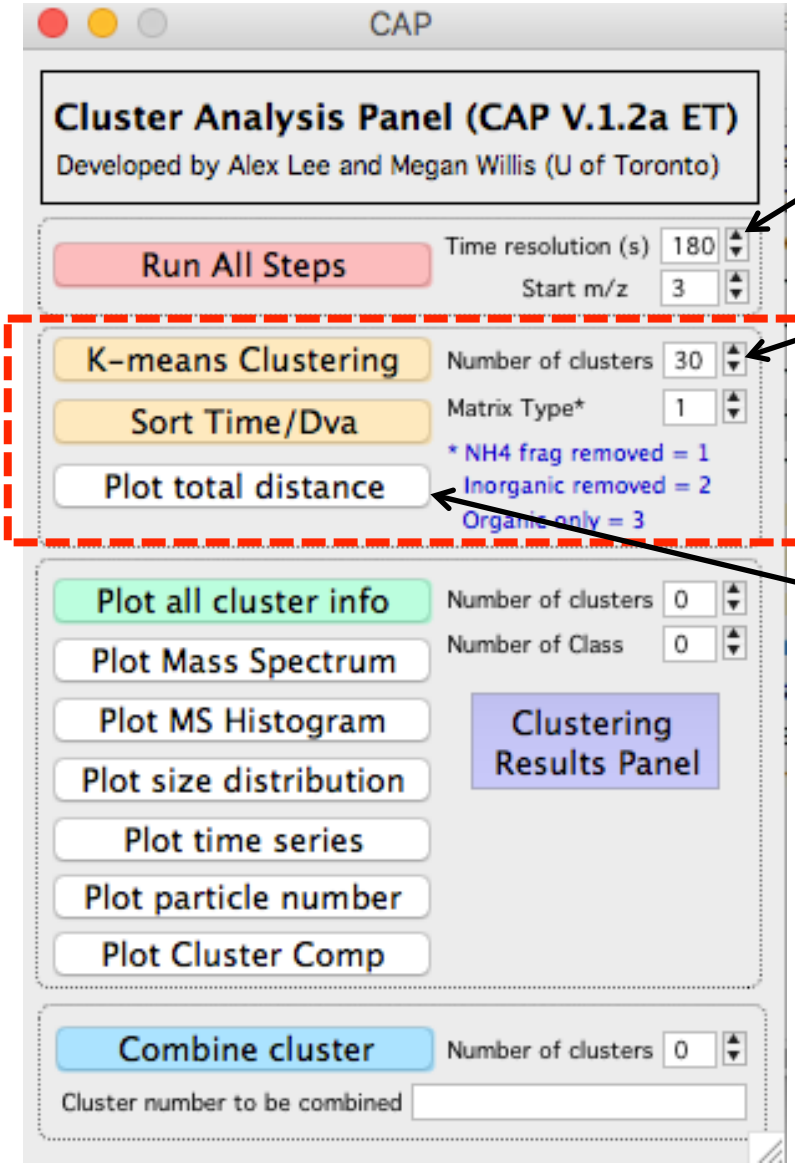
Results from CIPP



Ensemble vs. Event trigger data (smoothed)

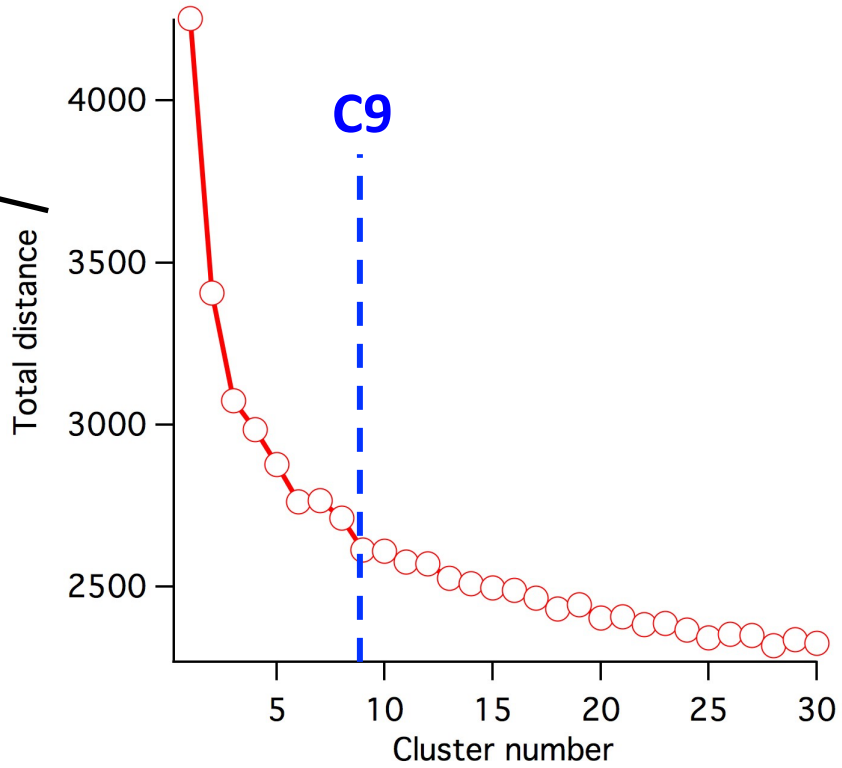


Cluster analysis Panel (CAP)

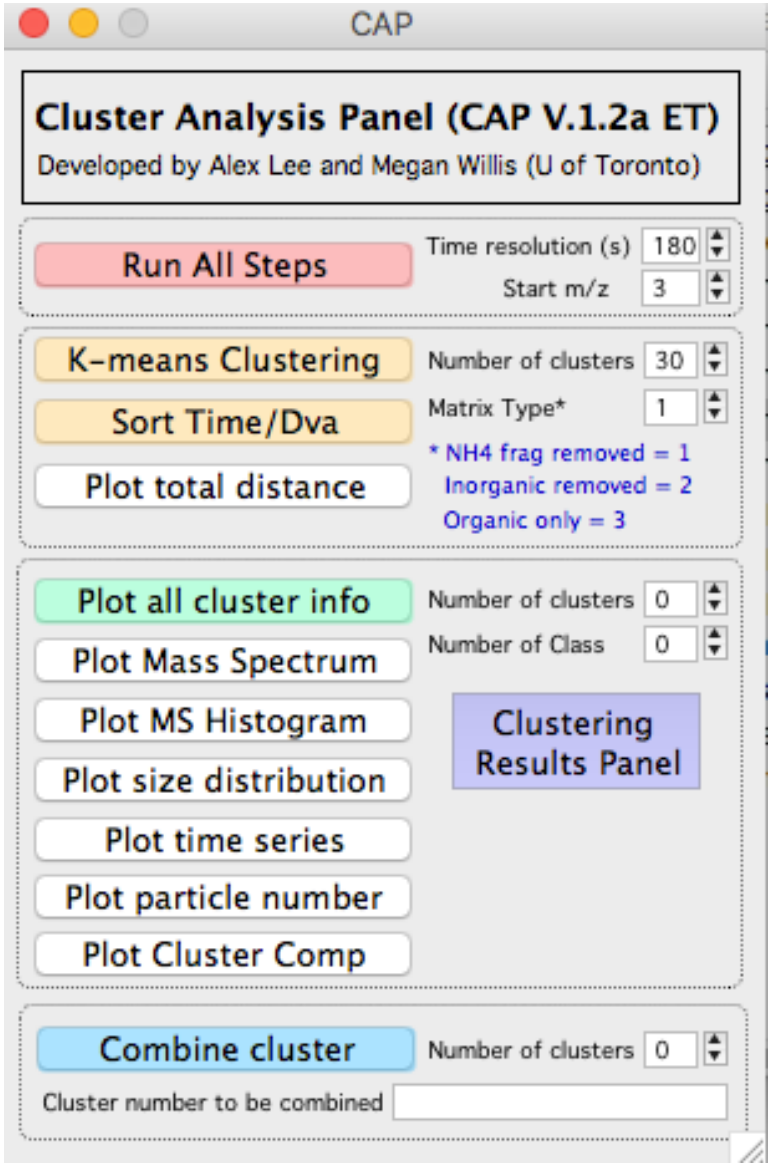


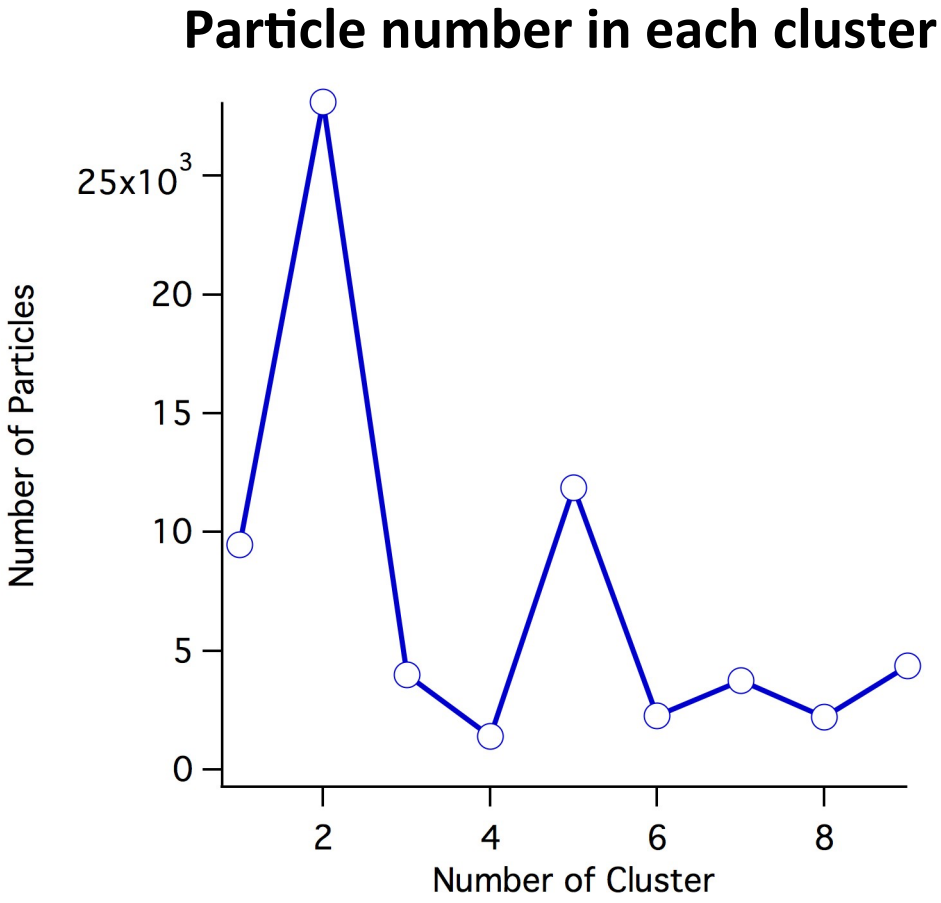
Time resolution (for plotting time series of event trigger data)

Number of cluster (Max = 30, built in k-means clustering from IGOR Pro)

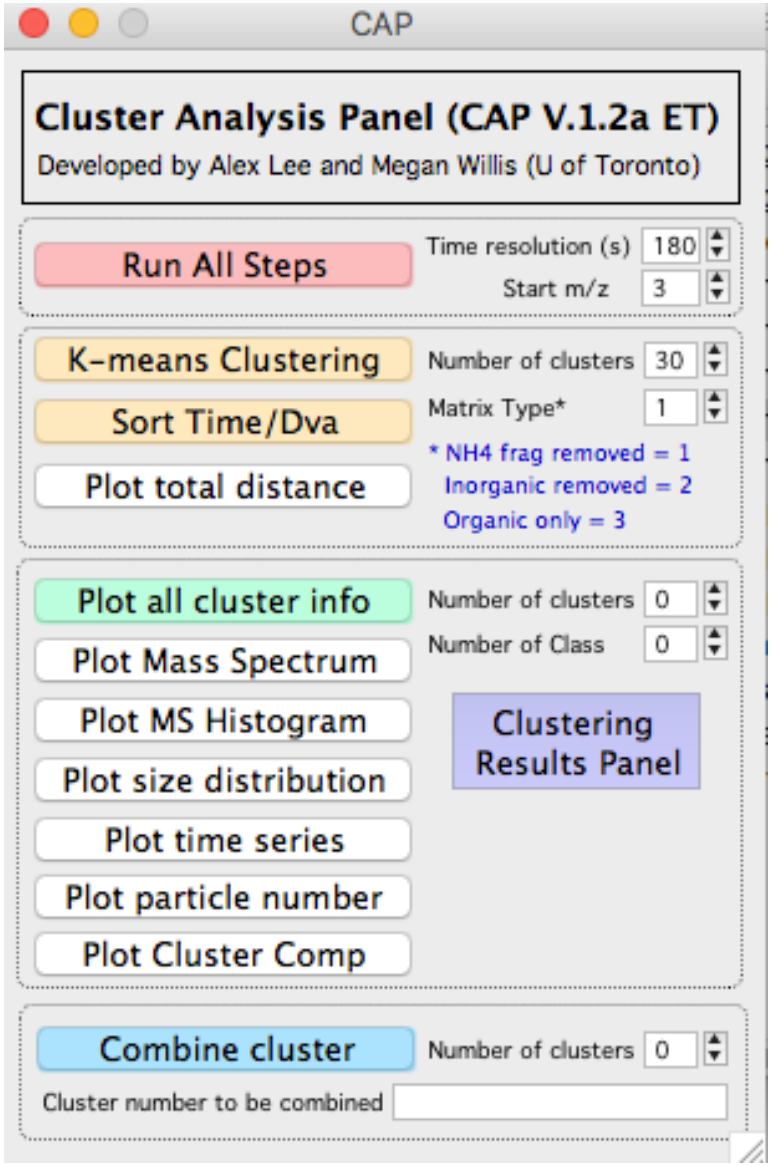


Cluster analysis Panel (CAP)

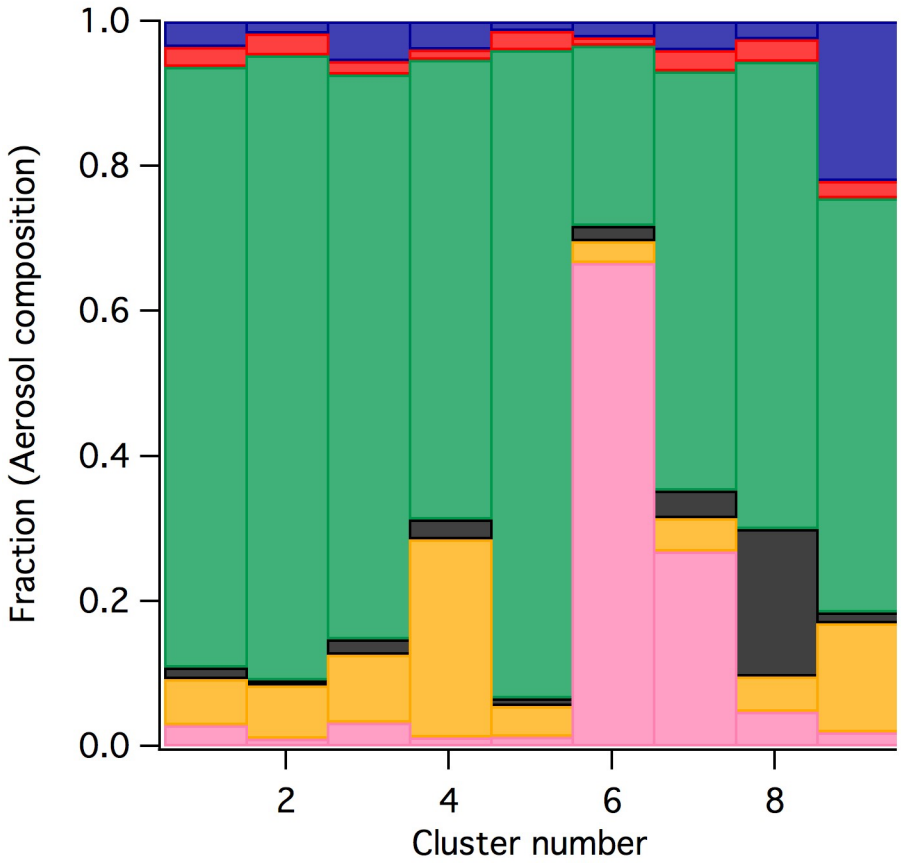




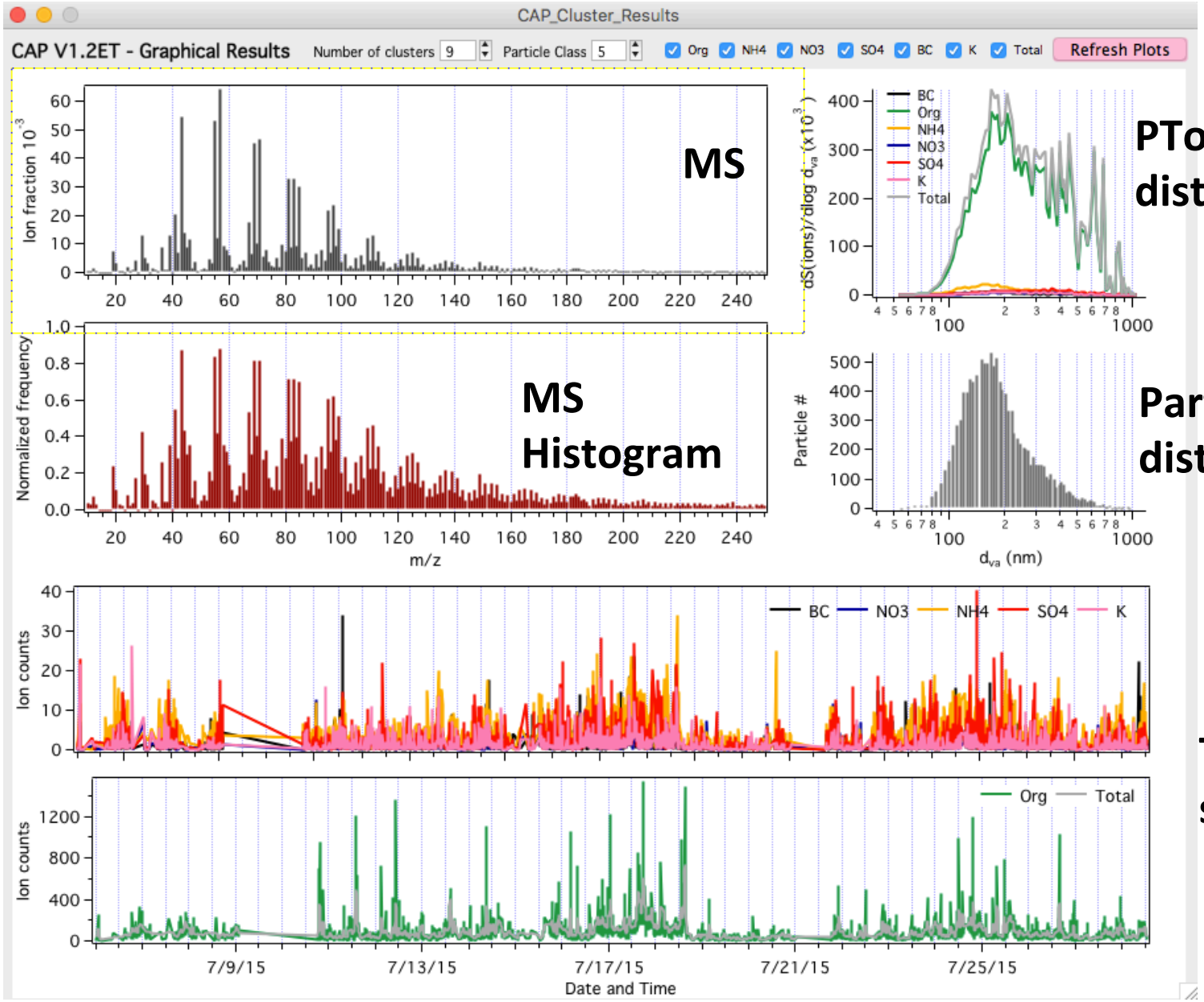
Cluster analysis Panel (CAP)



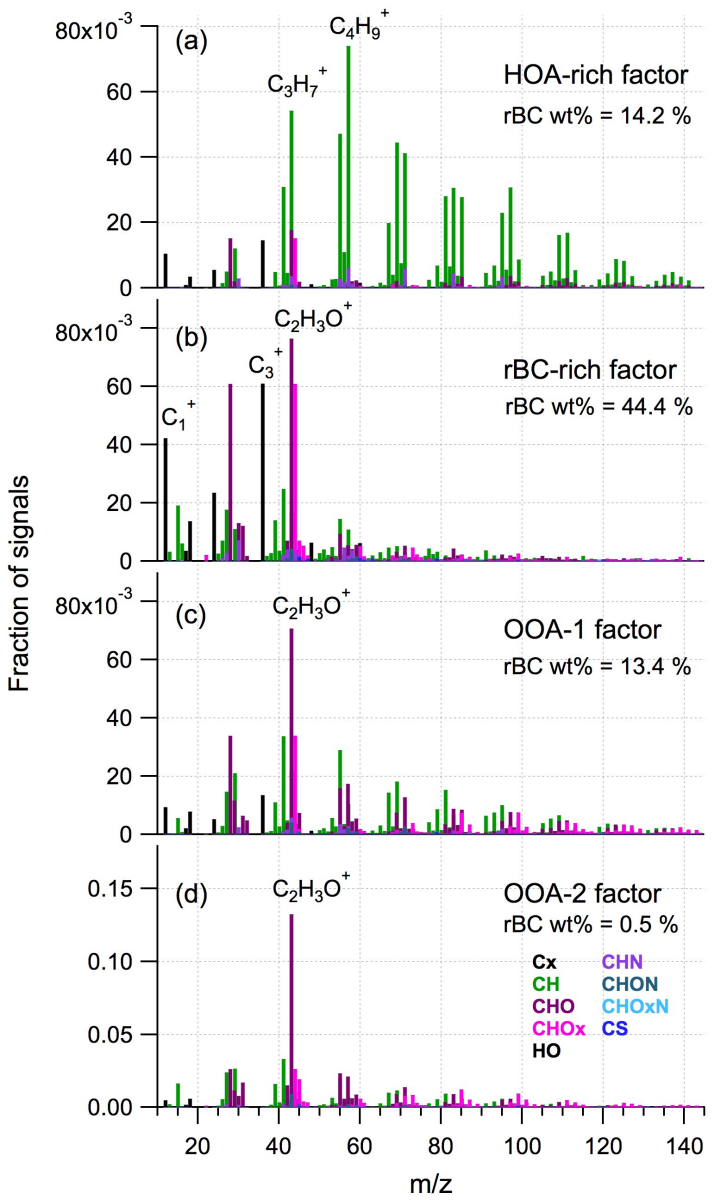
Fraction of ion signal in each cluster

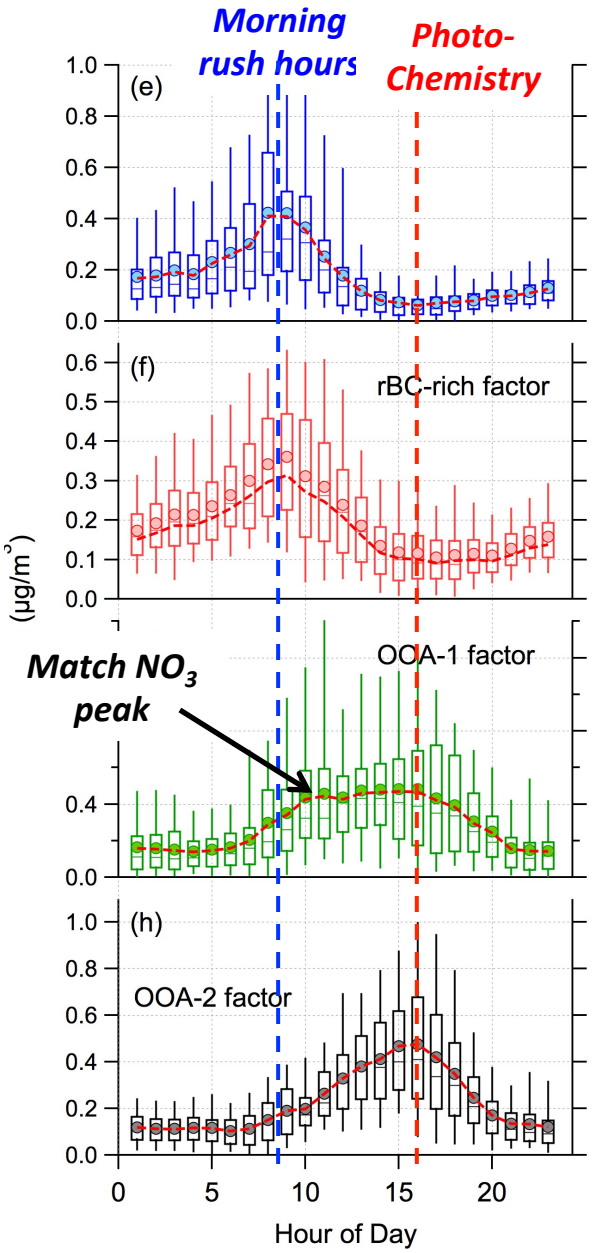


Graphical Results Panel



PMF analysis: 4-factors solution



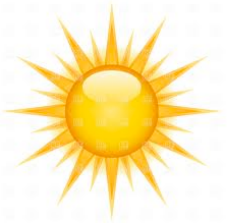


Hydrocarbon-like OA (HOA)-rich factor

rBC-rich factor

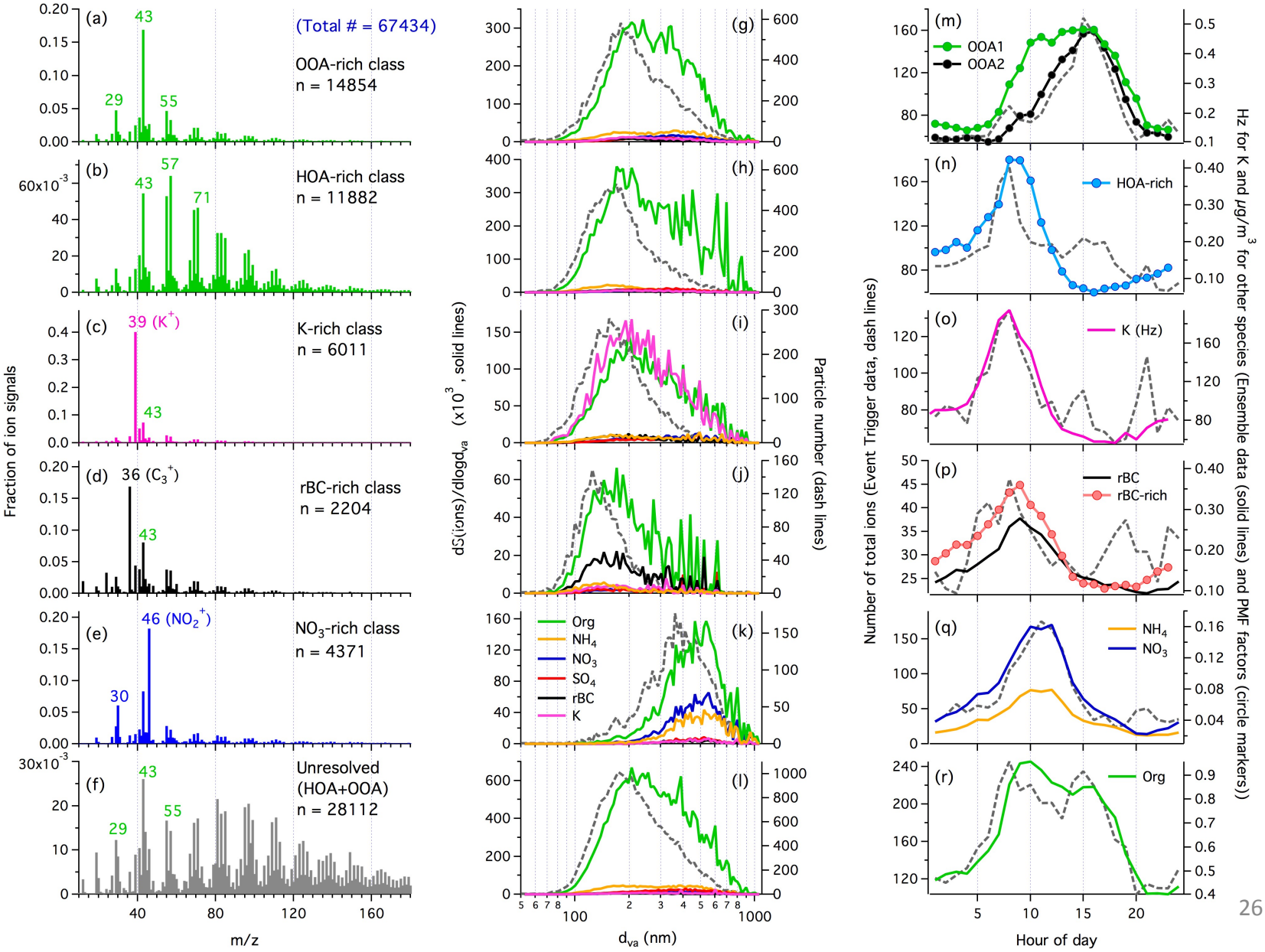
(with the support of single particle characterizations)

Oxygenated OA
OOA-1 factor

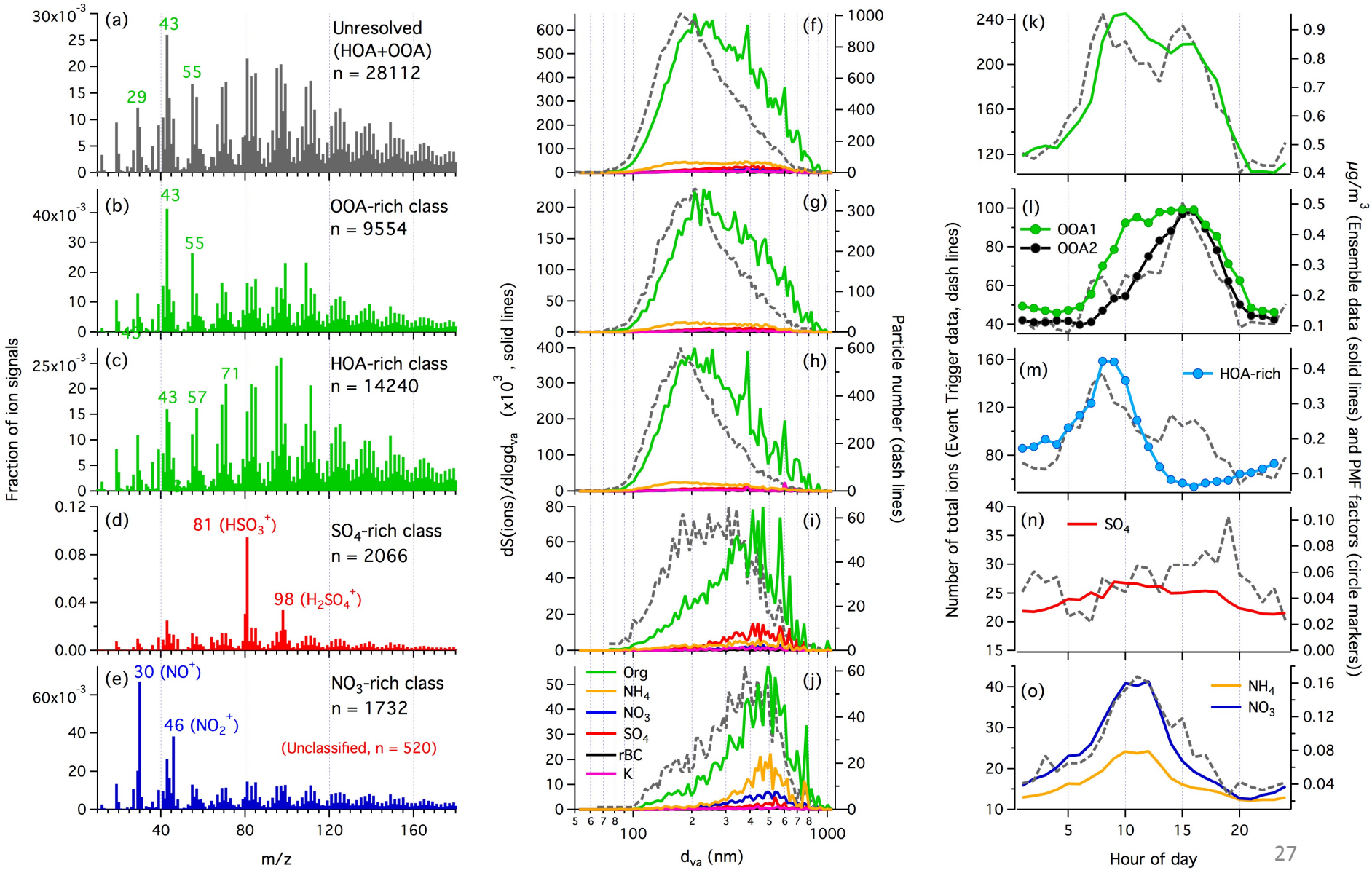


OOA-2 factor

Clustering results: 1st run (9-clusters solution)



Clustering results: 2nd run



Summary

- Remove false positive (improvement?)
- K-means clustering (works! Match PMF results)

- How to determine duty cycle for event trigger?
- Light scattering?