Characterization of Organic Aerosol Measured at the Centerville Ground Site by the Volatility and Polarity Separator (VAPS) during SOAS

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AMS Data Contributions from
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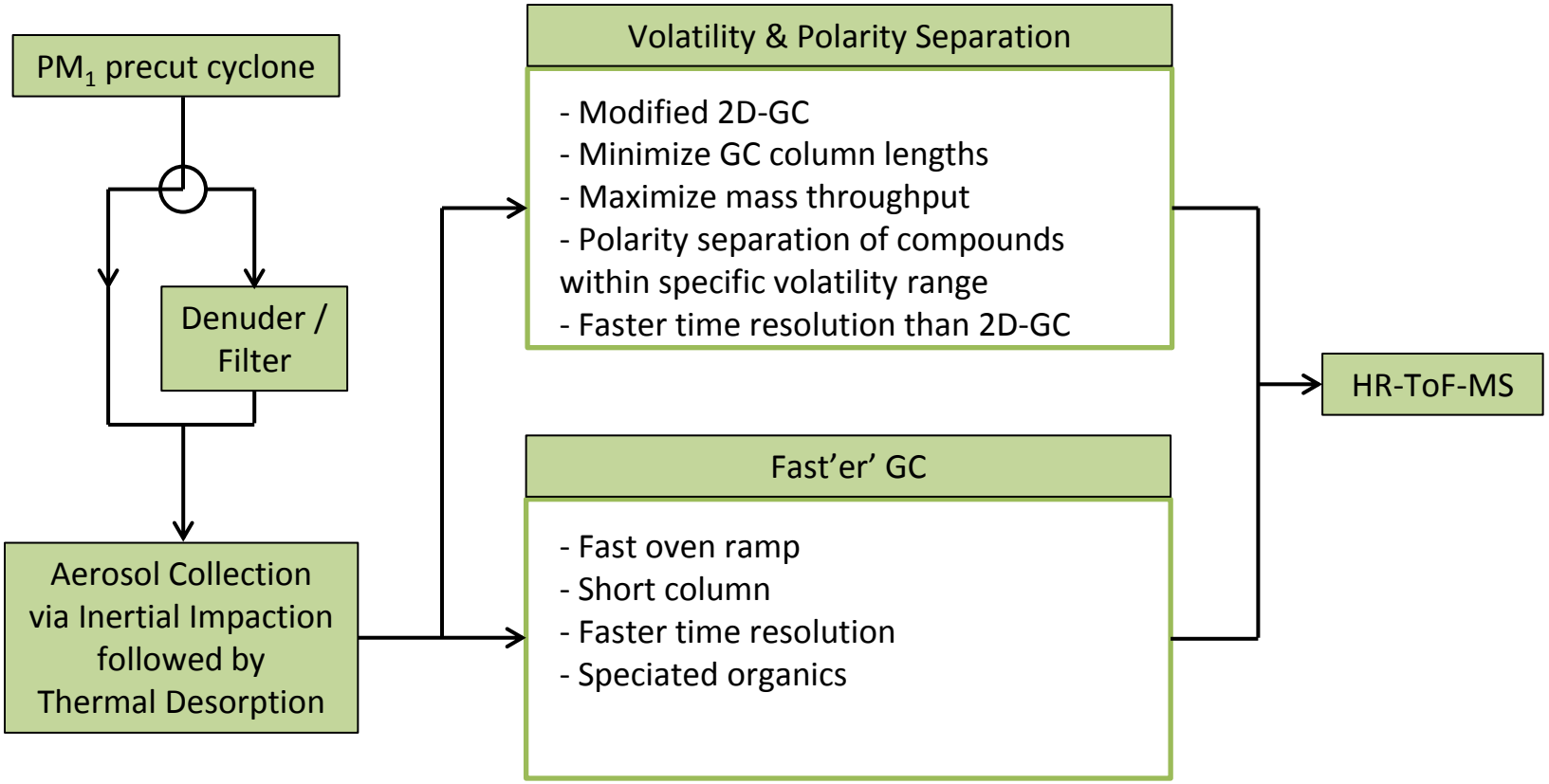
Motivation

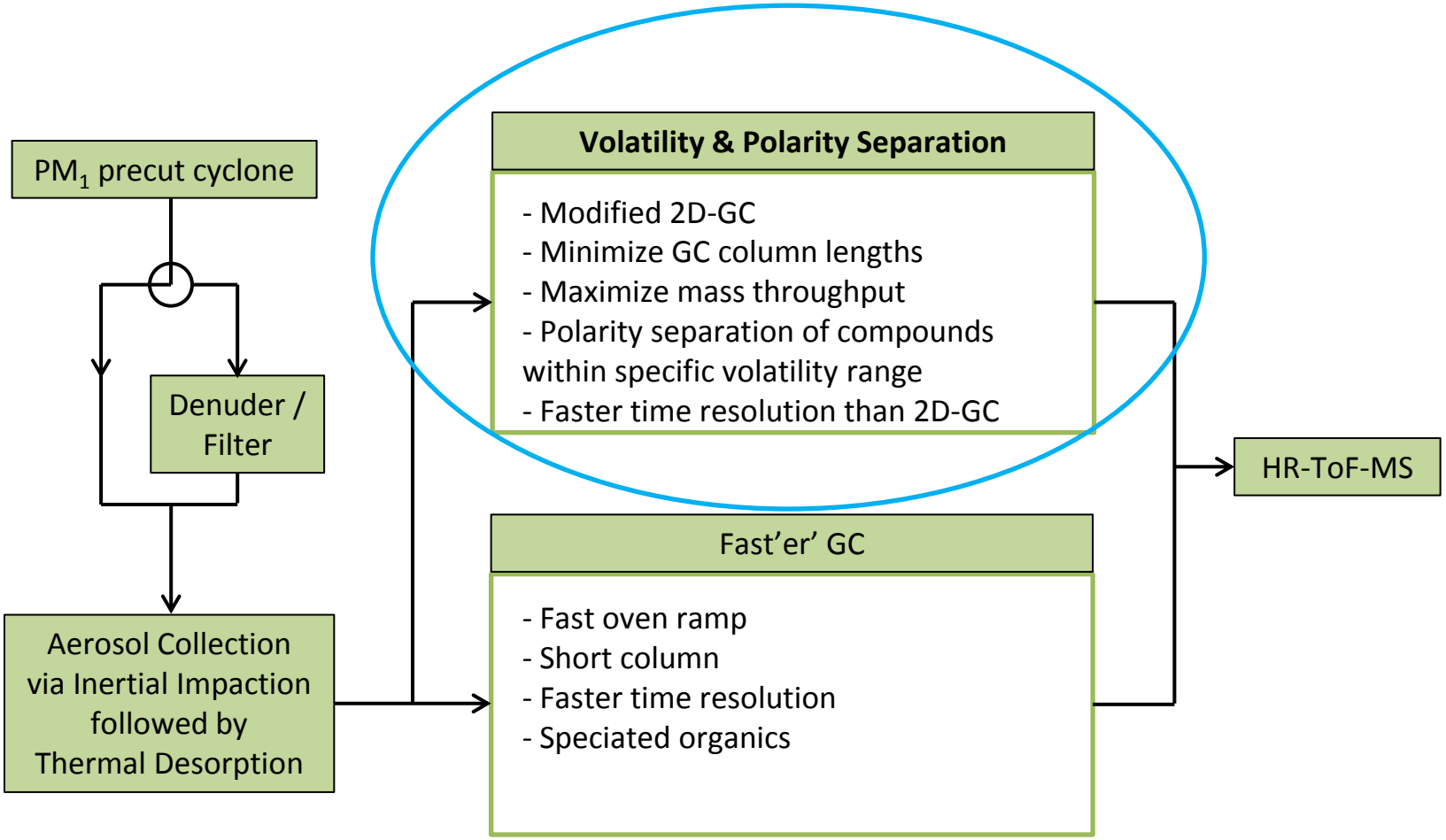
- Much uncertainty exists in the formation and evolution of OA
- Need for chemical insights on anthropogenically influenced biogenic SOA
- Need new manageable parameterizations of this chemistry

Located at Centerville Ground Site

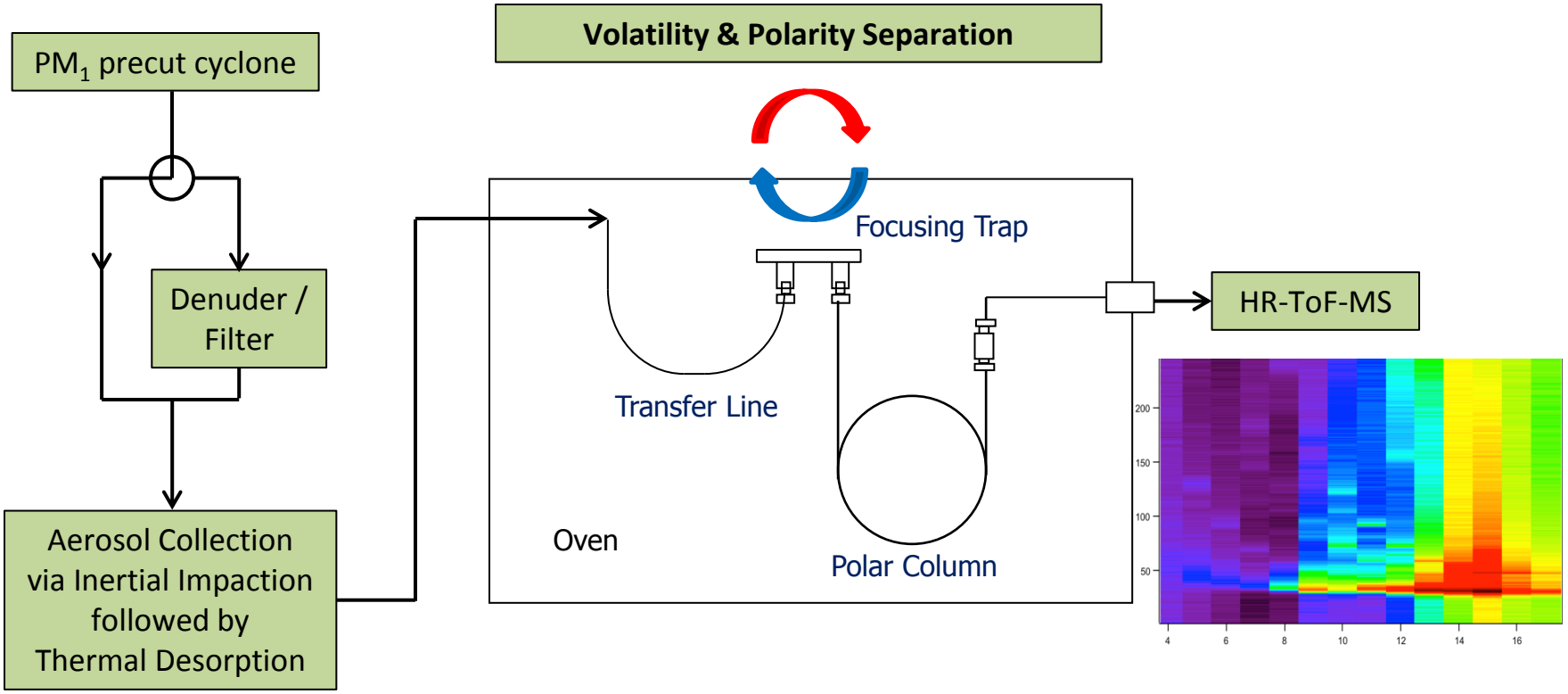
The Volatility & Polarity Separator (VAPS)



Mode 1: Volatility & Polarity Separation



Mode 1: Volatility & Polarity Separation



OA Evolution & 2D Representation

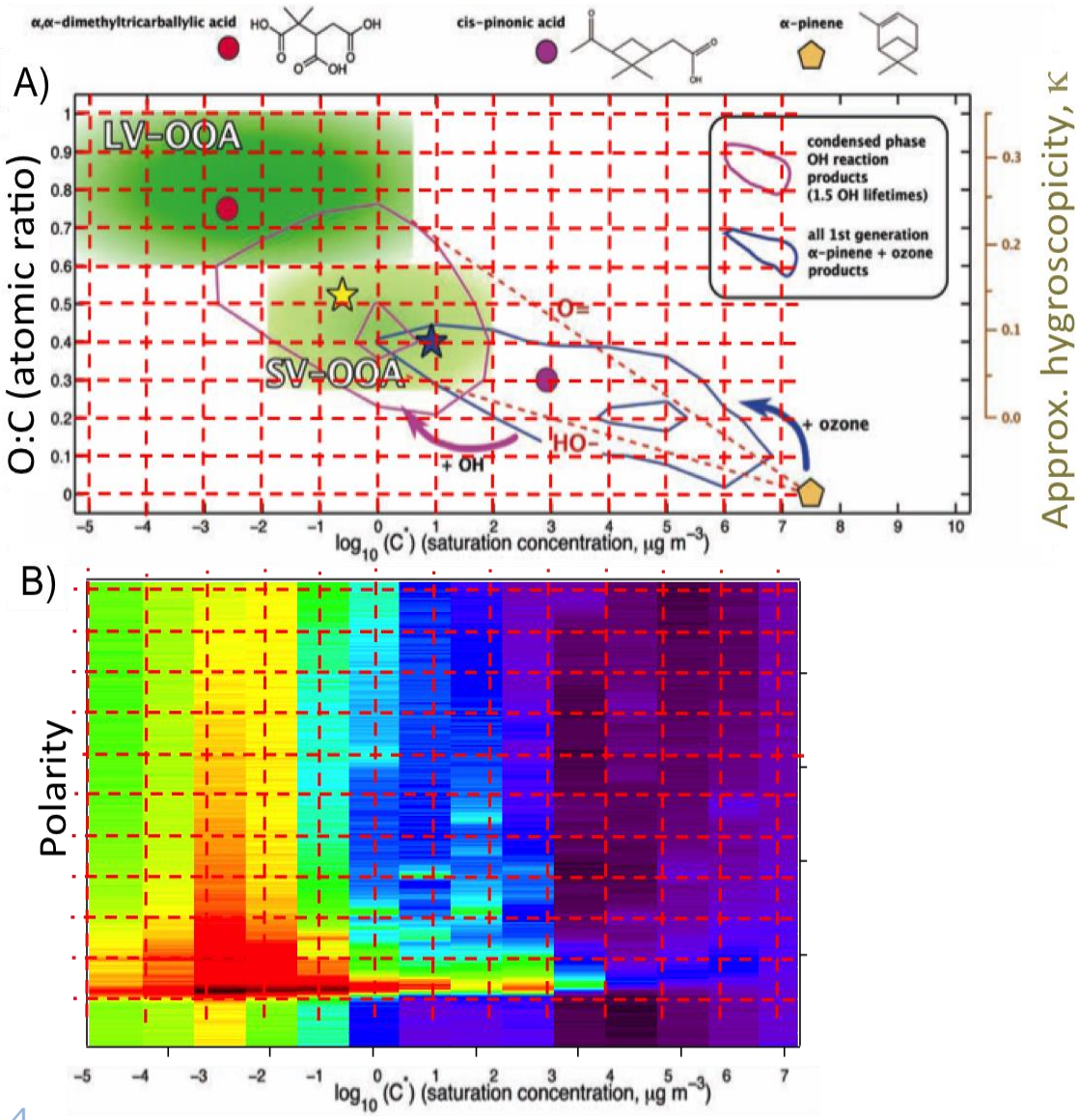


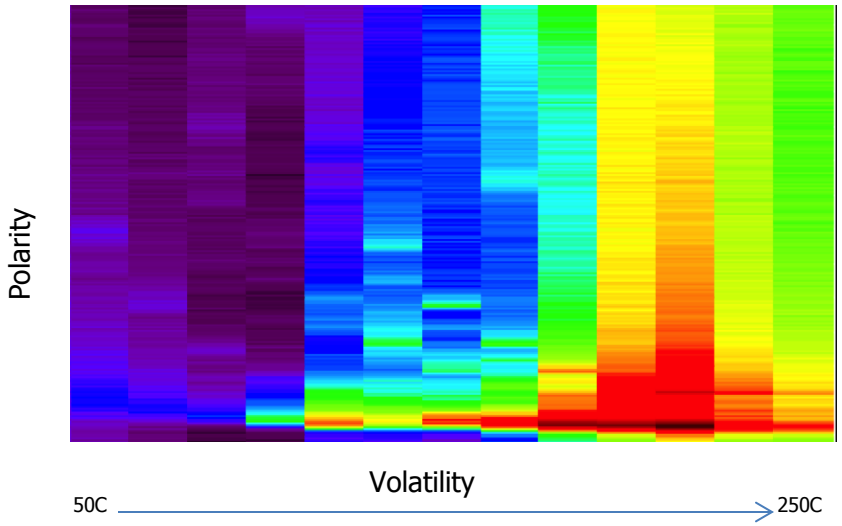
Illustration of SOA evolution through 2D-VBS space

Jimenez et al., Science, 2009

Ambient VAPS sample from St. Louis, MO.

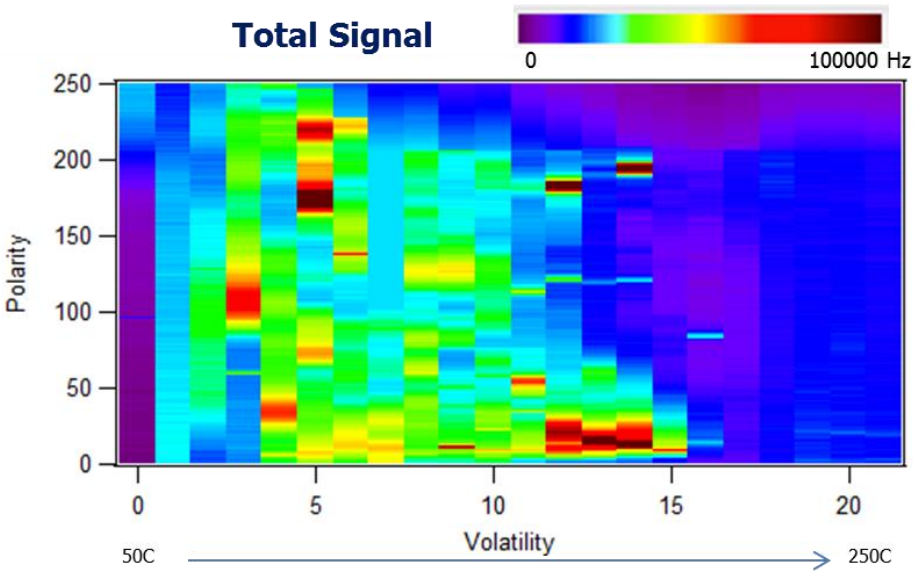
Present are alkanes, moncarboxylic acids, dicarboxylic acids, ketones, aldehydes, PAHs, oxy-PAHs, phthalates, and fatty acid methyl esters.

2D Polarity vs Volatility Plot



Ambient VAPS sample from St. Louis, MO.

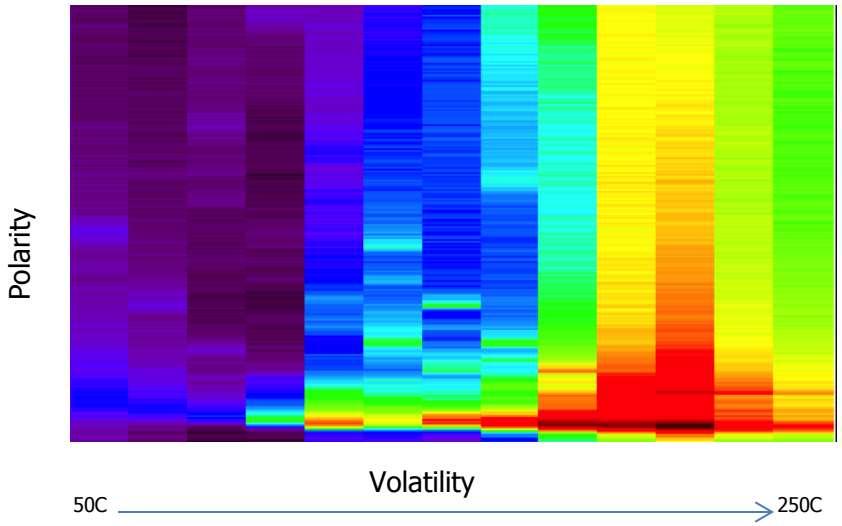
2D Polarity vs Volatility Plot



SOAS Sample

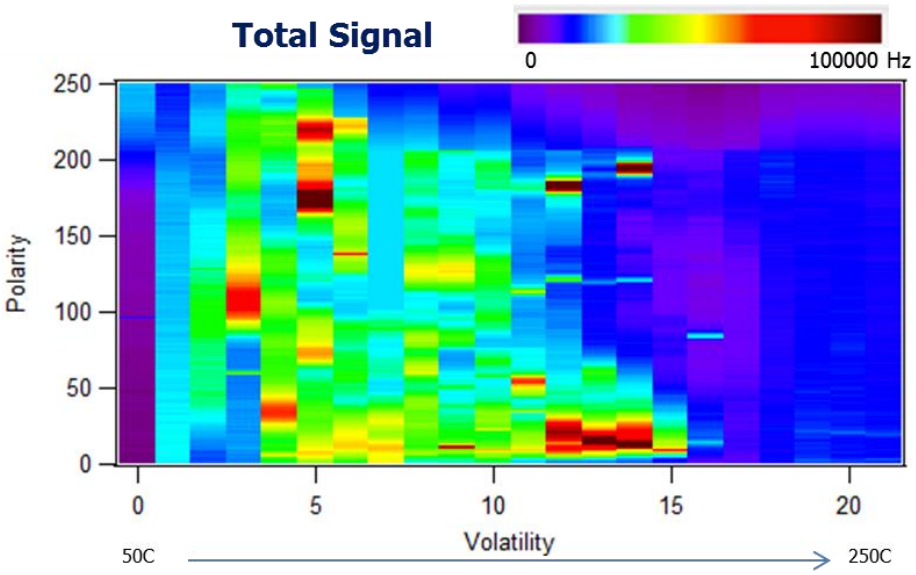
Sample Date:
06/17/13

Sample Time:
9:09am – 9:39am

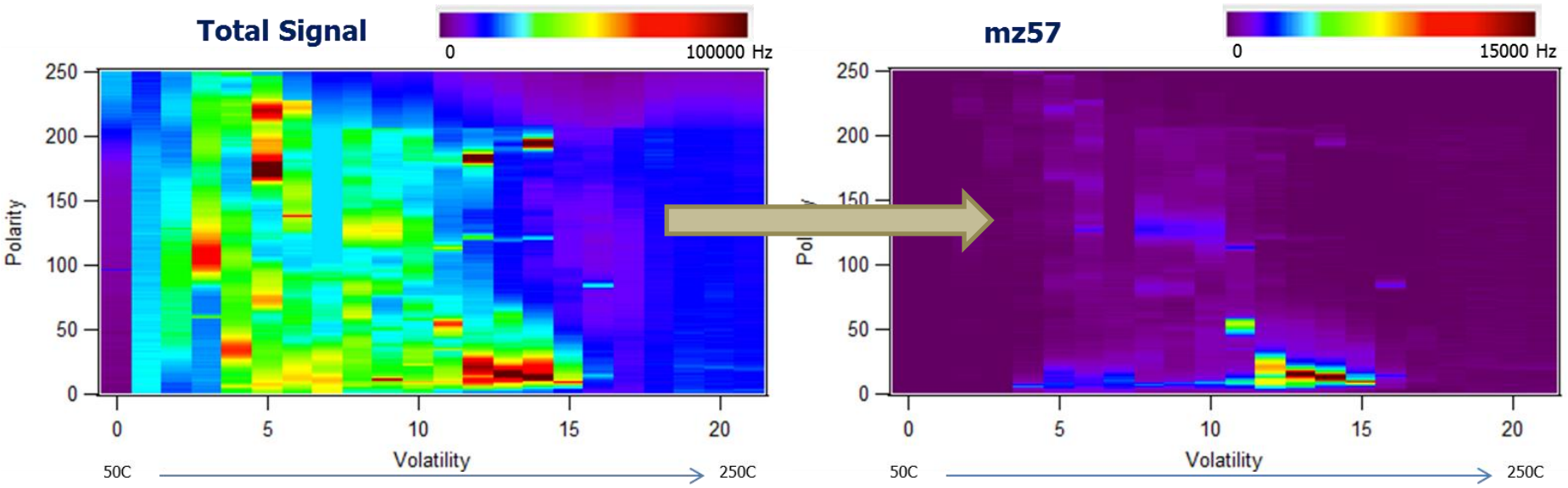


Ambient VAPS sample from St. Louis, MO.

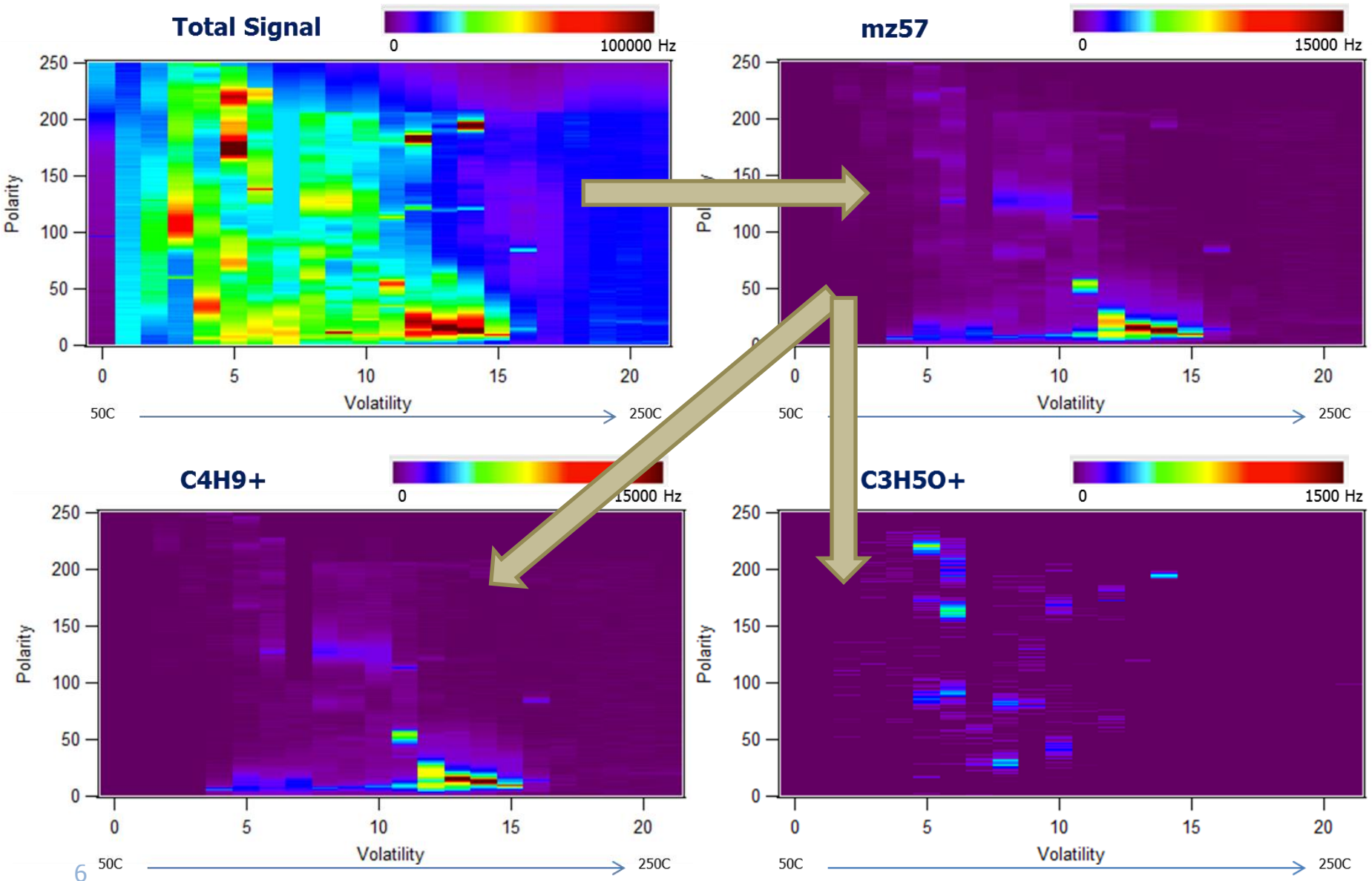
2D Polarity vs Volatility Plot



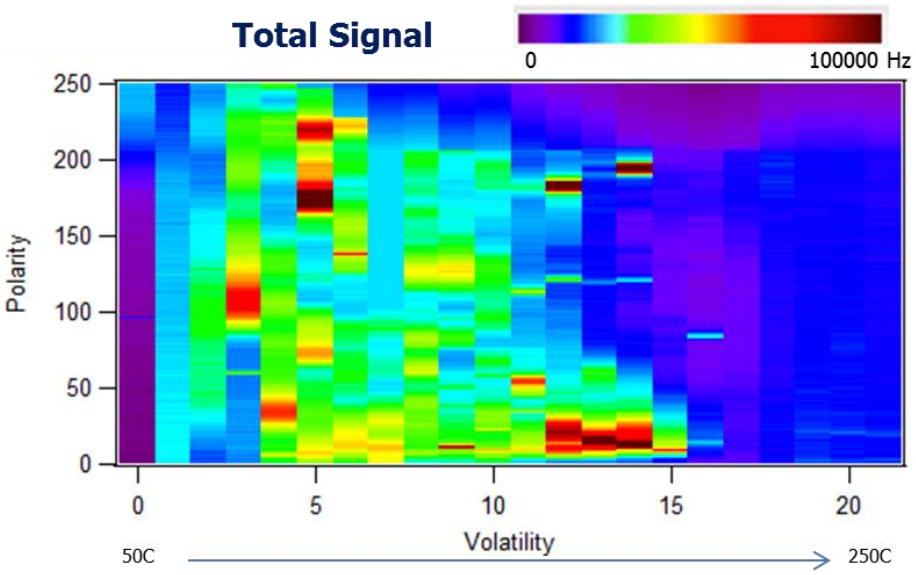
2D Polarity vs Volatility Plot



2D Polarity vs Volatility Plot



2D Polarity vs Volatility Plot



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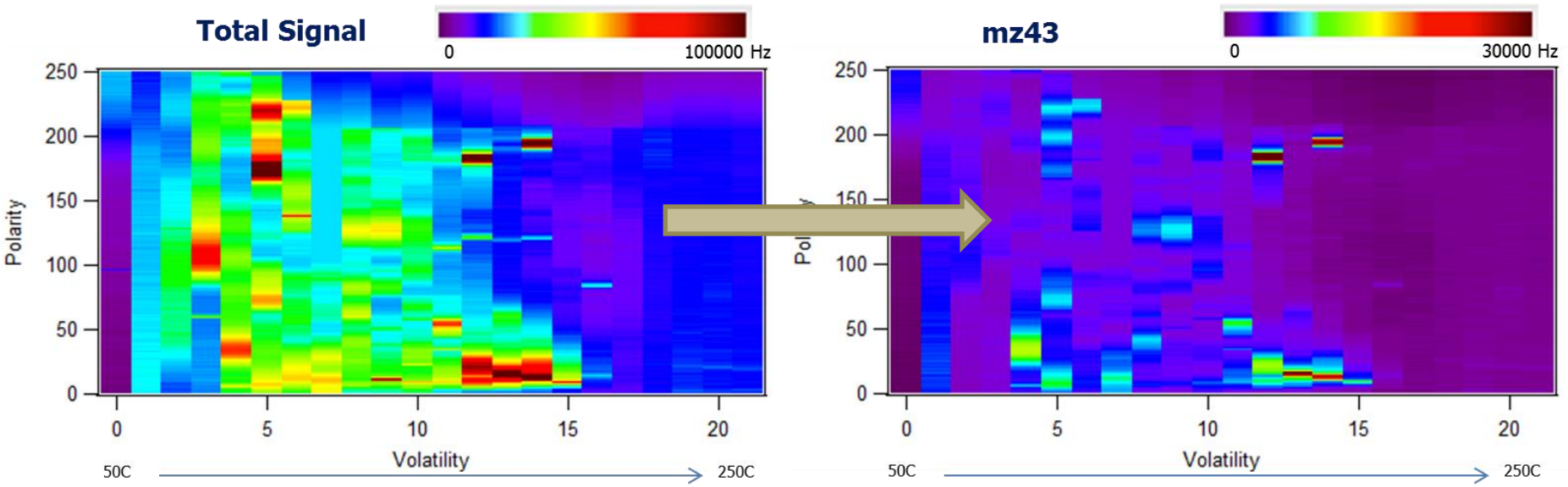
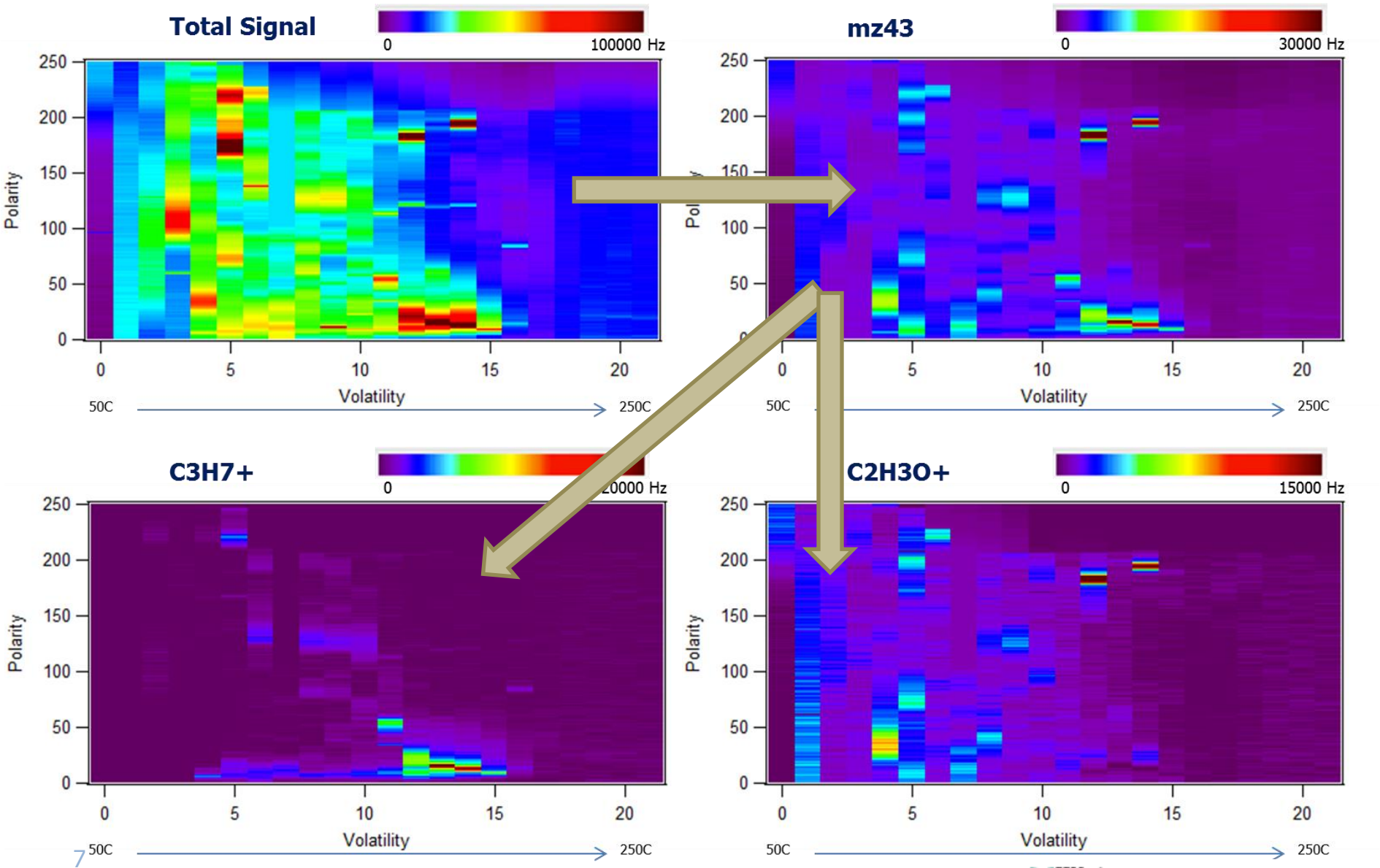
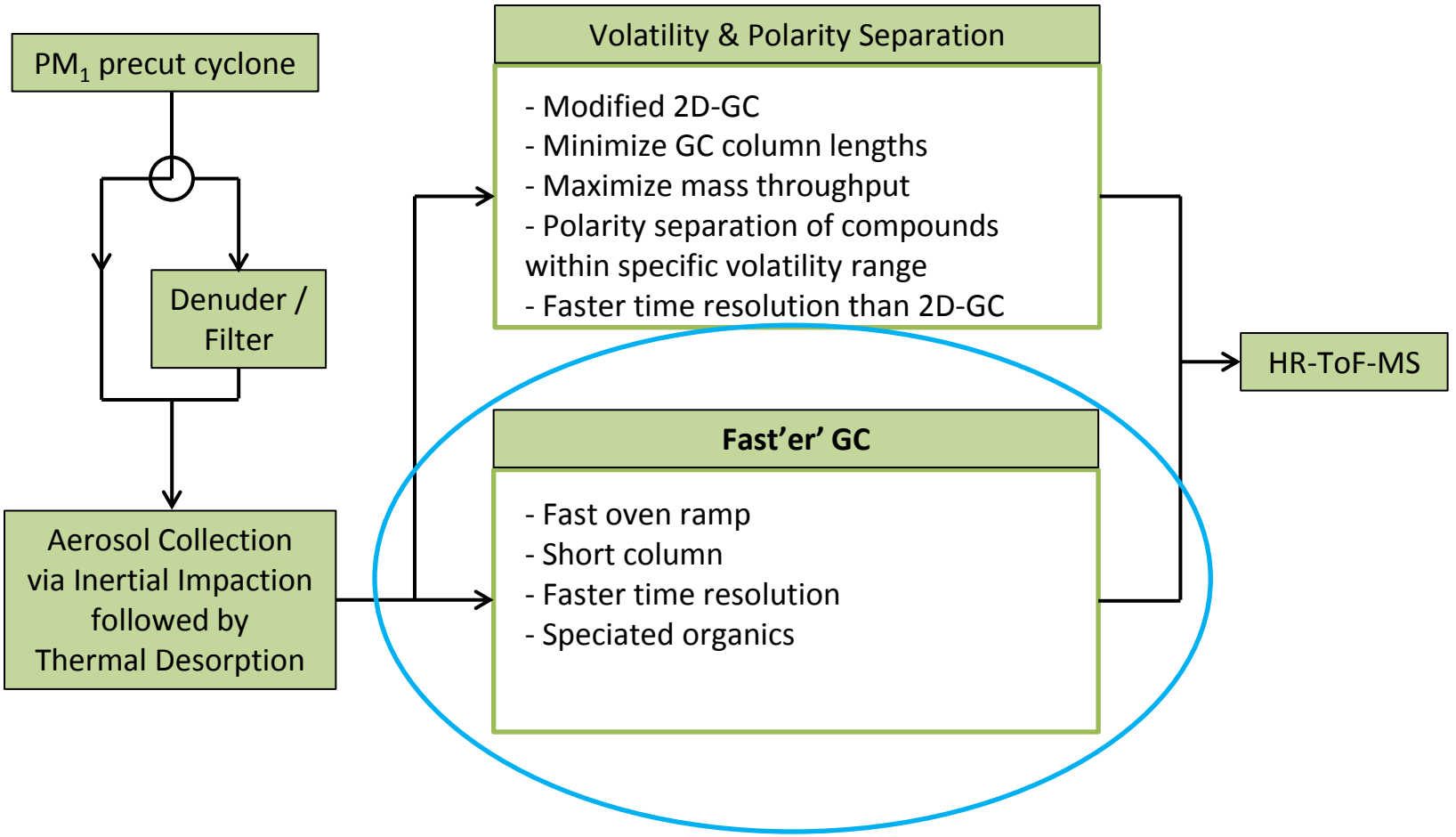


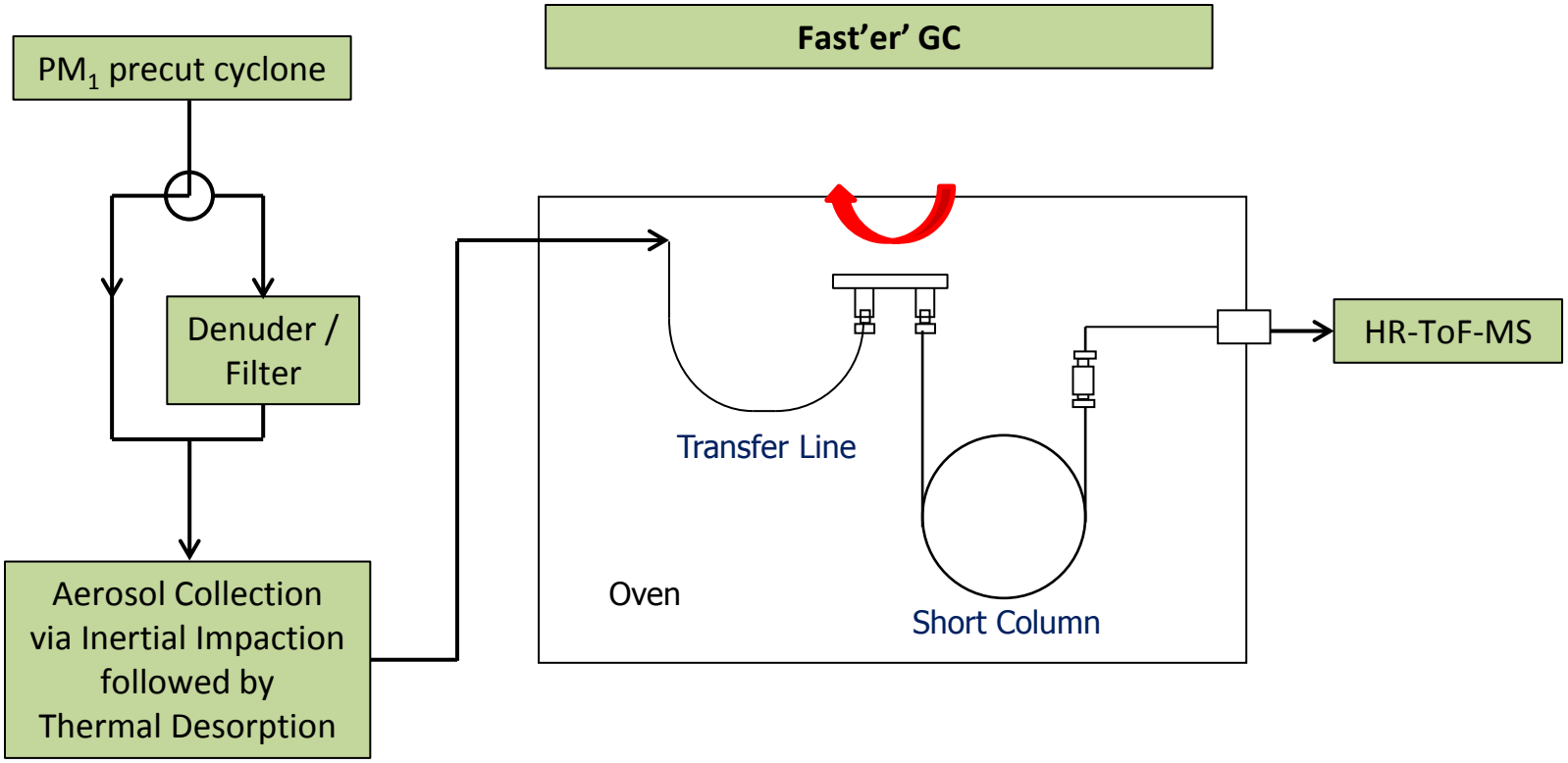
2D Polarity vs Volatility Plot



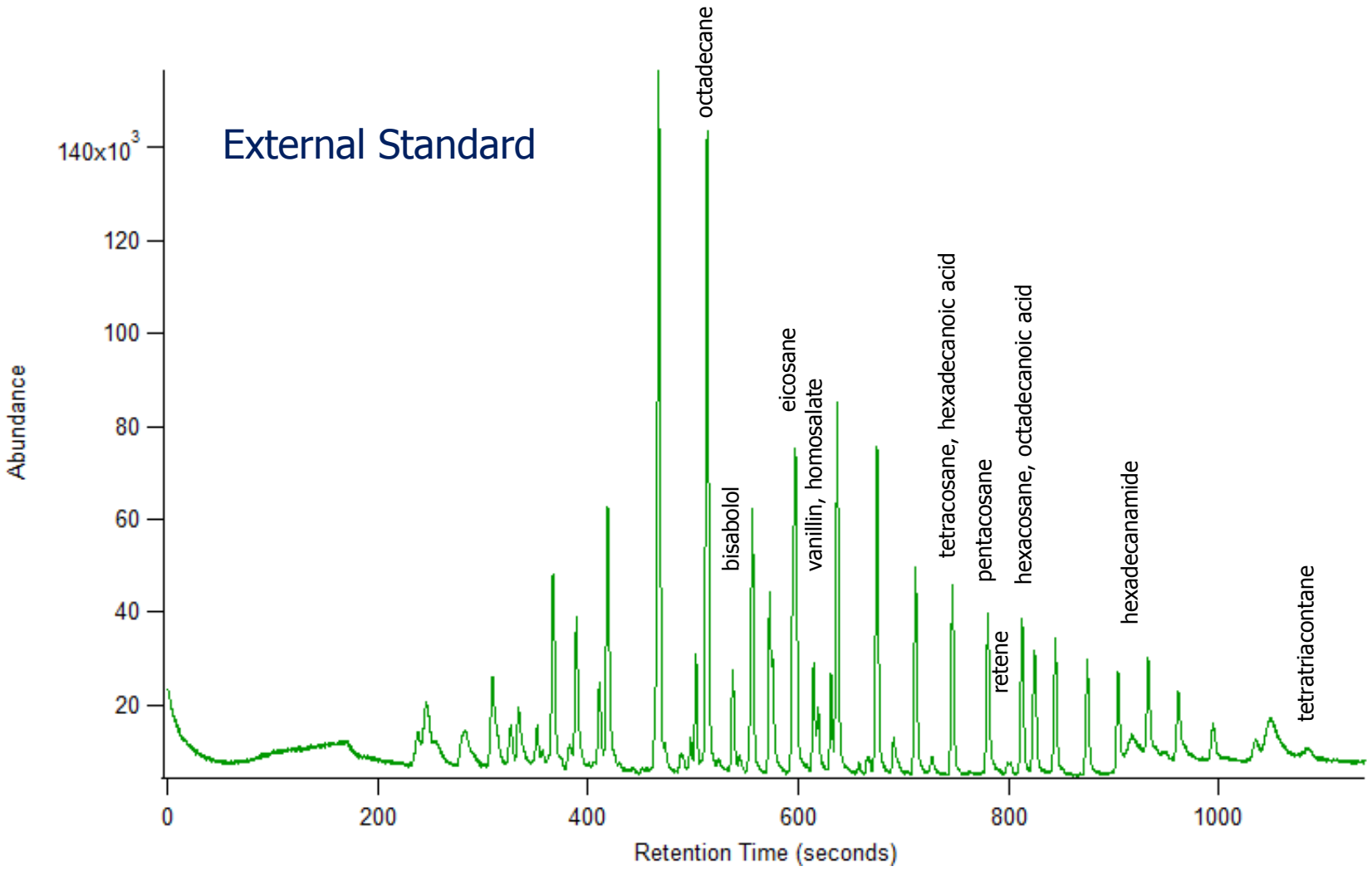
Mode 2: Fast'er' GC



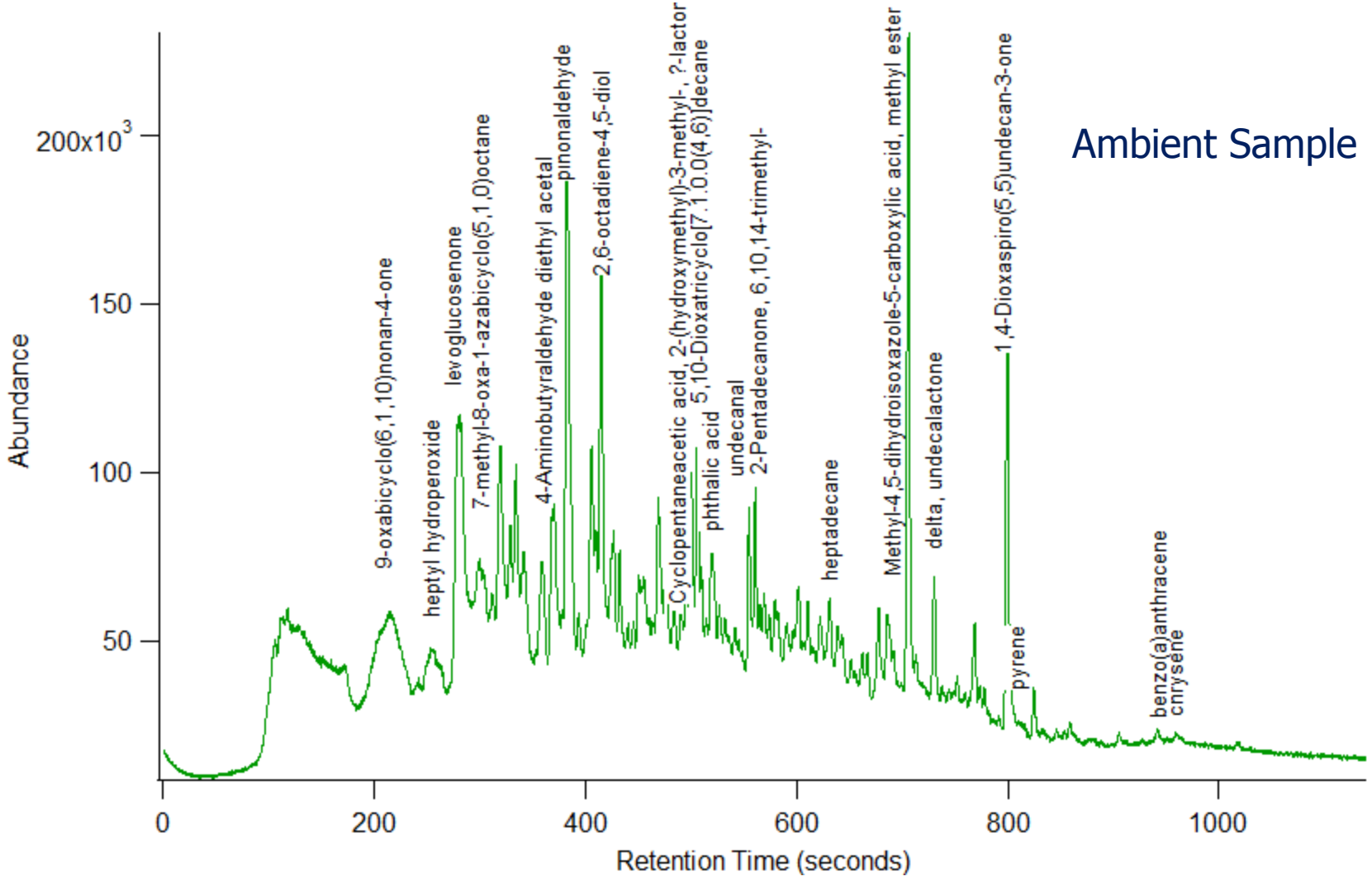
Mode 2: Fast'er' GC



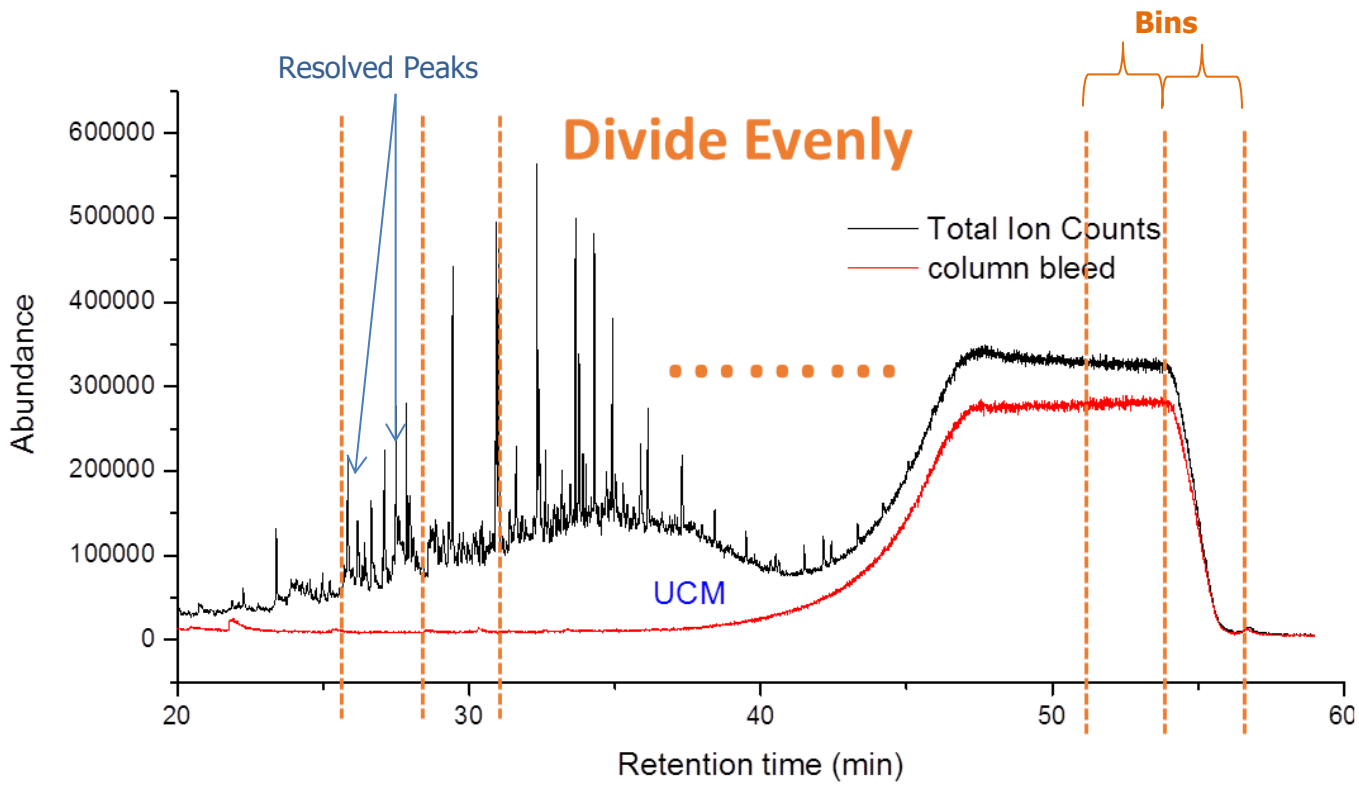
VAPS Fast'er' GC Chromatogram



VAPS Fast'er' GC Chromatogram

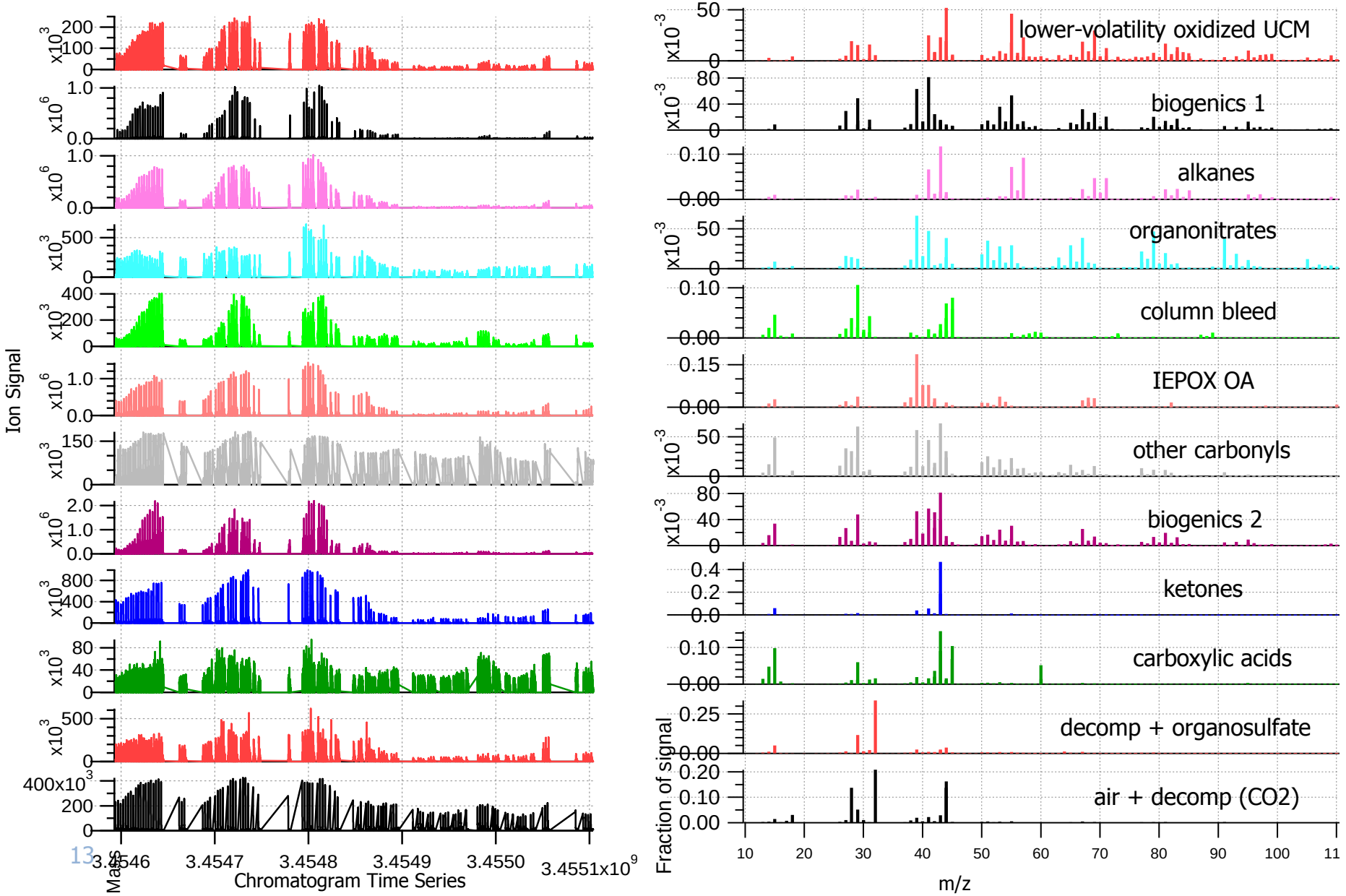


PMF on Binned Chromatogram

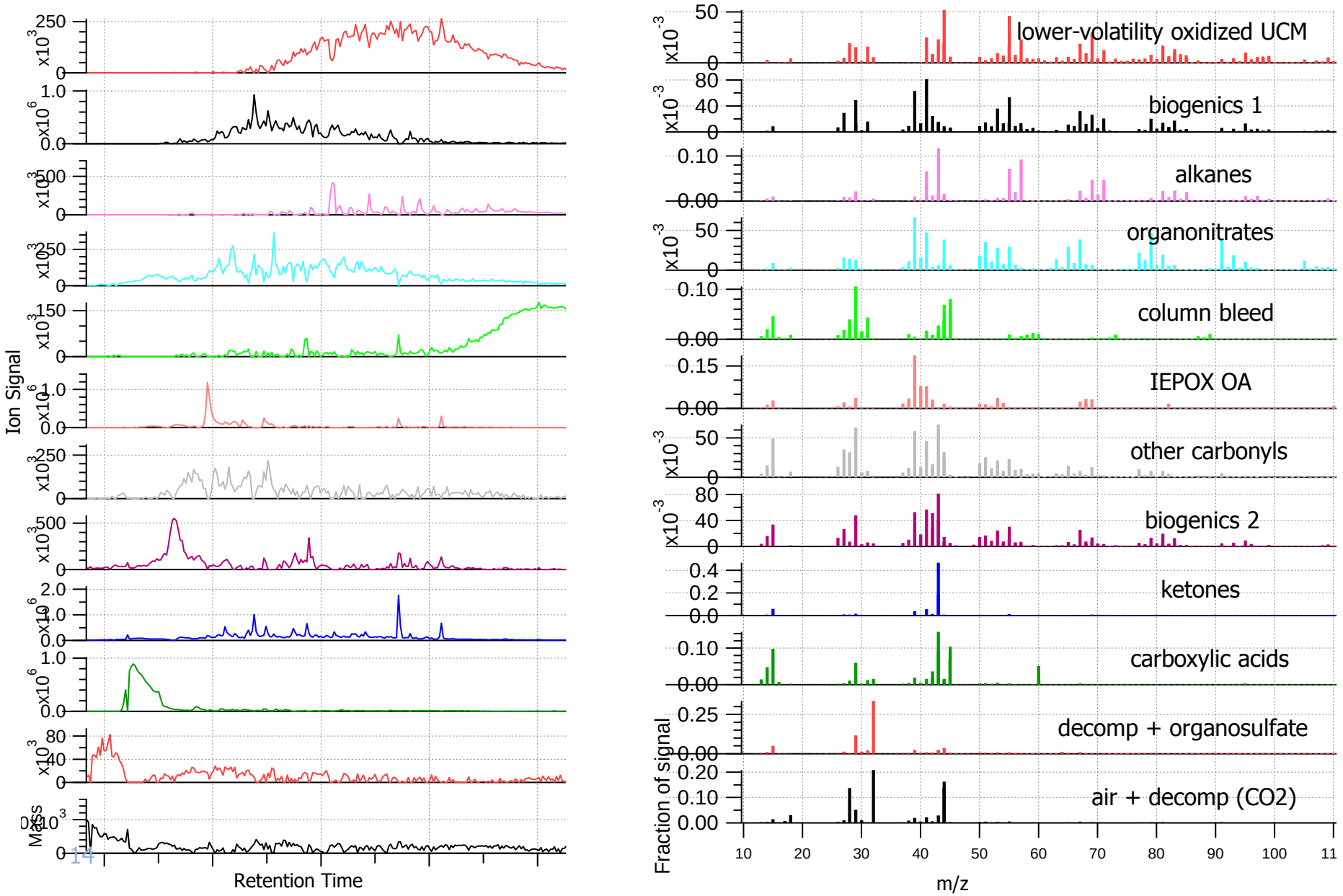


Zhang et al, AS&T, submitted

PMF – Hi Res – 12 Factors



PMF – Hi Res – 12 Factors



Correlation with AMS Factors

AMS PMF Factors

VAPS PMF Factors

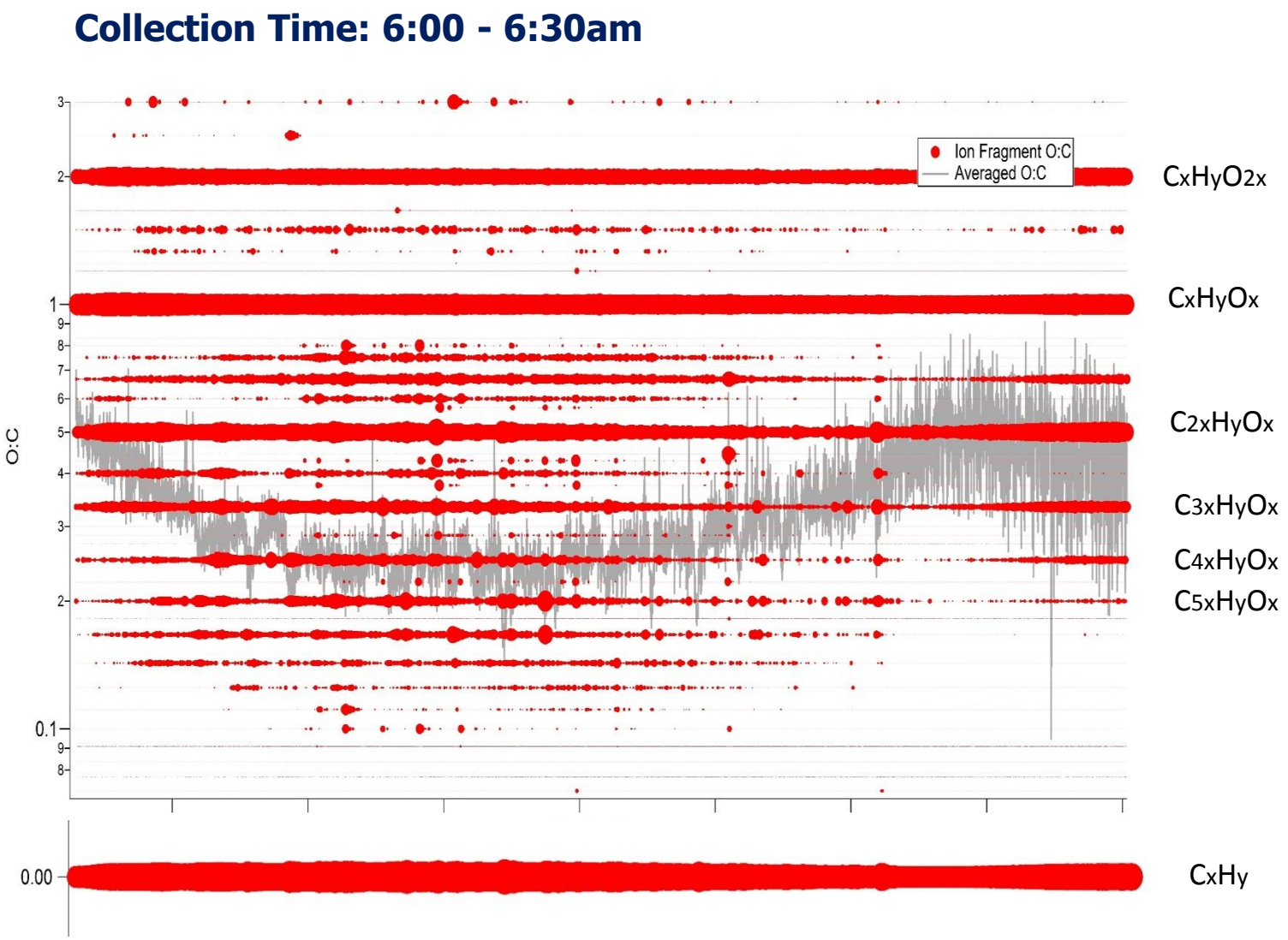
	IEPOX	LVOOA	SVOOA	BBOA
air + decomp	-	-	-	-
decomp + organosulfate	-	-	-	-
carboxylic acids	0.64	0.85	0.86	0.85
ketones	-	0.72	0.92	0.82
biogenics 2	-	0.78	0.91	0.82
other carbonyls	-	0.80	0.65	0.81
IEPOX OA	0.62	0.80	0.90	0.86
organonitrates	-	-	0.91	0.74
alkanes	-	-	-	-
biogenics 1	-	0.75	0.90	0.84
lower volatility oxidized UCM	-	0.70	0.93	0.84

AMS Factors from Lu Xu, Sally Ng, Georgia Tech

other approach to interpreting data

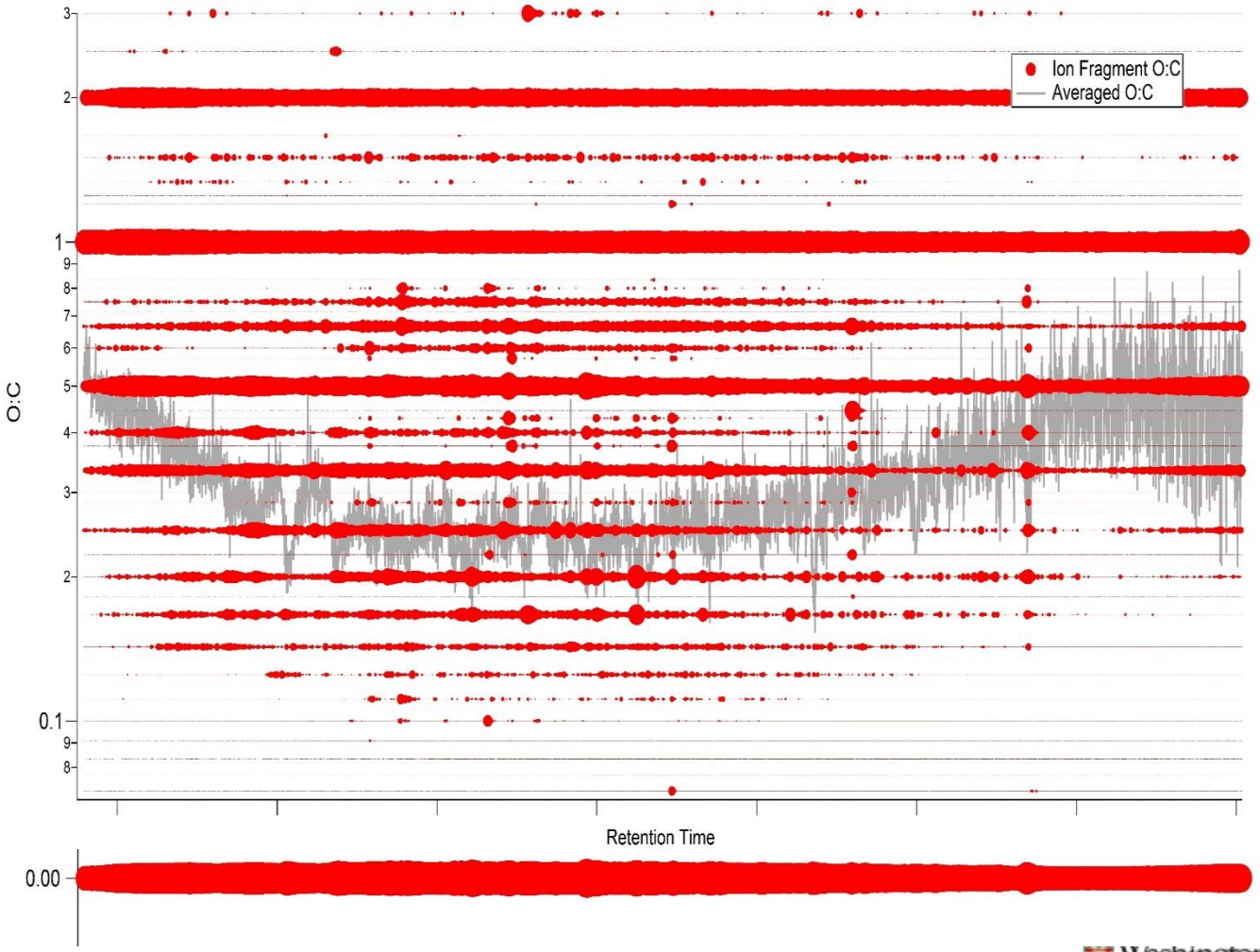
O:C (Ion Fragments) versus Retention Time

formula	O:C
CxHyO3x	3
C2HyO5	2.5
CxHyO2x	2
C3HyO5	1.67
C2xHyO3x	1.5
C3HyO4	1.33
C4HyO5	1.25
C5HyO6	1.2
CxHyOx	1
C6HyO5	0.83
C5HyO4	0.8
C4HyO3	0.75
C7HyO5	0.71
C3xHyO2x	0.67
C5HyO3	0.6
C7HyO4	0.57
C2xHyOx	0.5
C9HyO4	0.44
C7H7O3	0.43
C5xHyO2x	0.4
C8HyO3	0.38
C3xHyOx	0.33
C10HyO3	0.3
C7HyO2	0.29
C11HyO3	0.27
C4xHyOx	0.25
C9HyO2	0.22
C5xHyOx	0.2
C11HyO2	0.18
C6xHyOx	0.17
C7HyO	0.14
C8HyO	0.13
C9HyO	0.11
C10HyO	0.1
C11HyO	0.09
C12HyO	0.08
C13HyO	0.08
C14HyO	0.07
CxHy	0



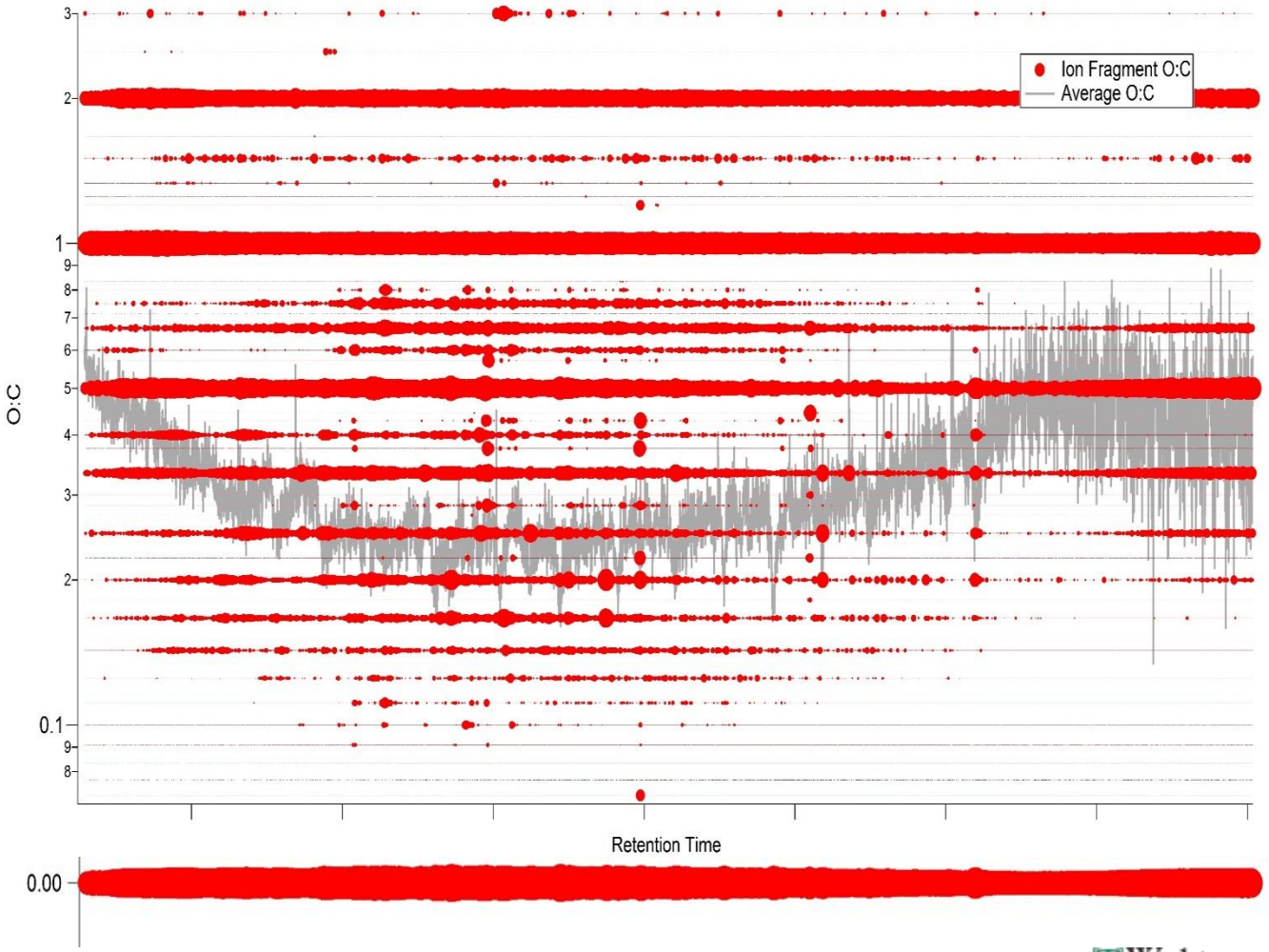
O:C (Ion Fragments) versus Retention Time

Collection Time: 6:45 – 7:15am



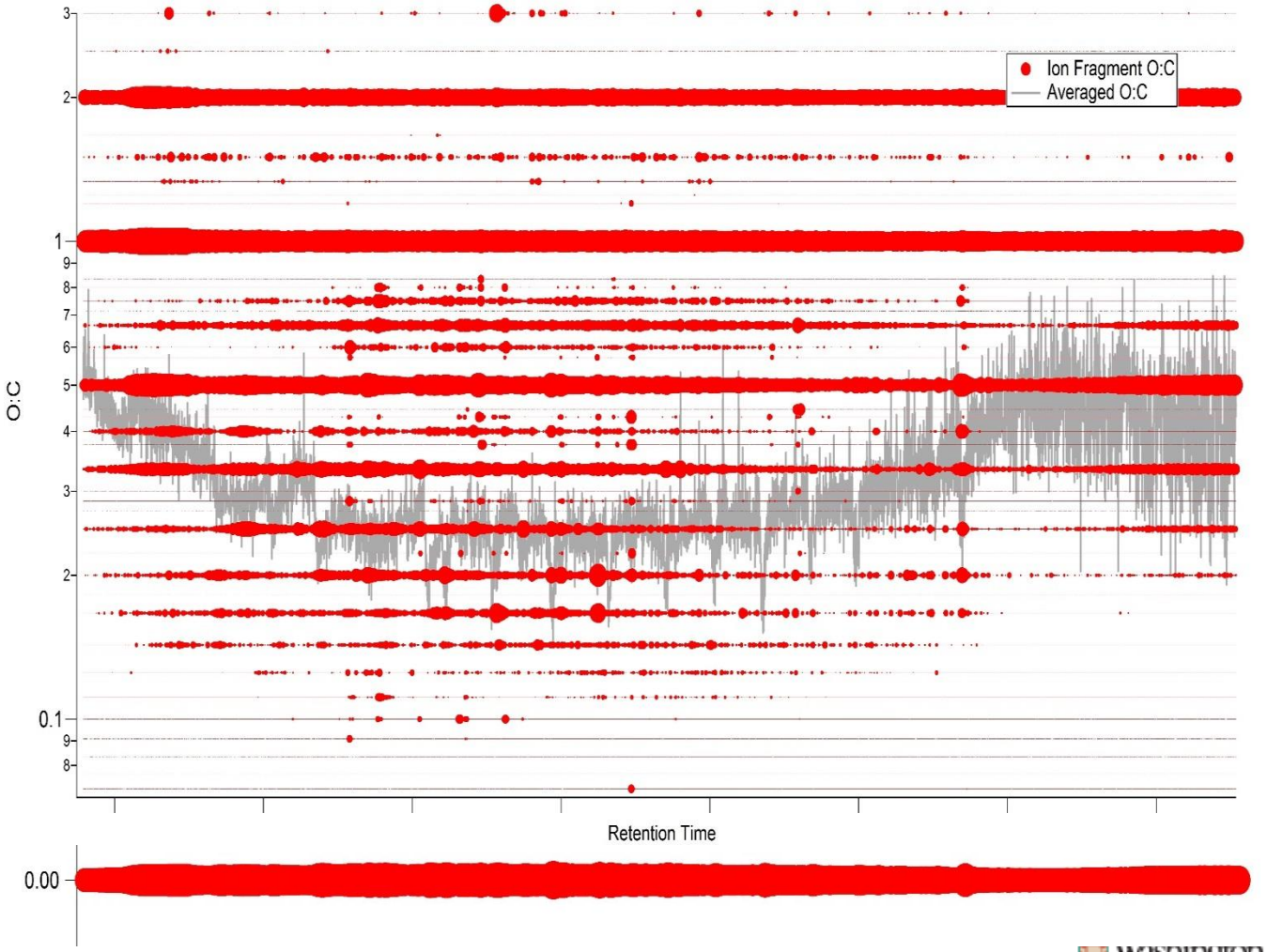
O:C (Ion Fragments) versus Retention Time

Collection Time: 7:30 – 8:00am



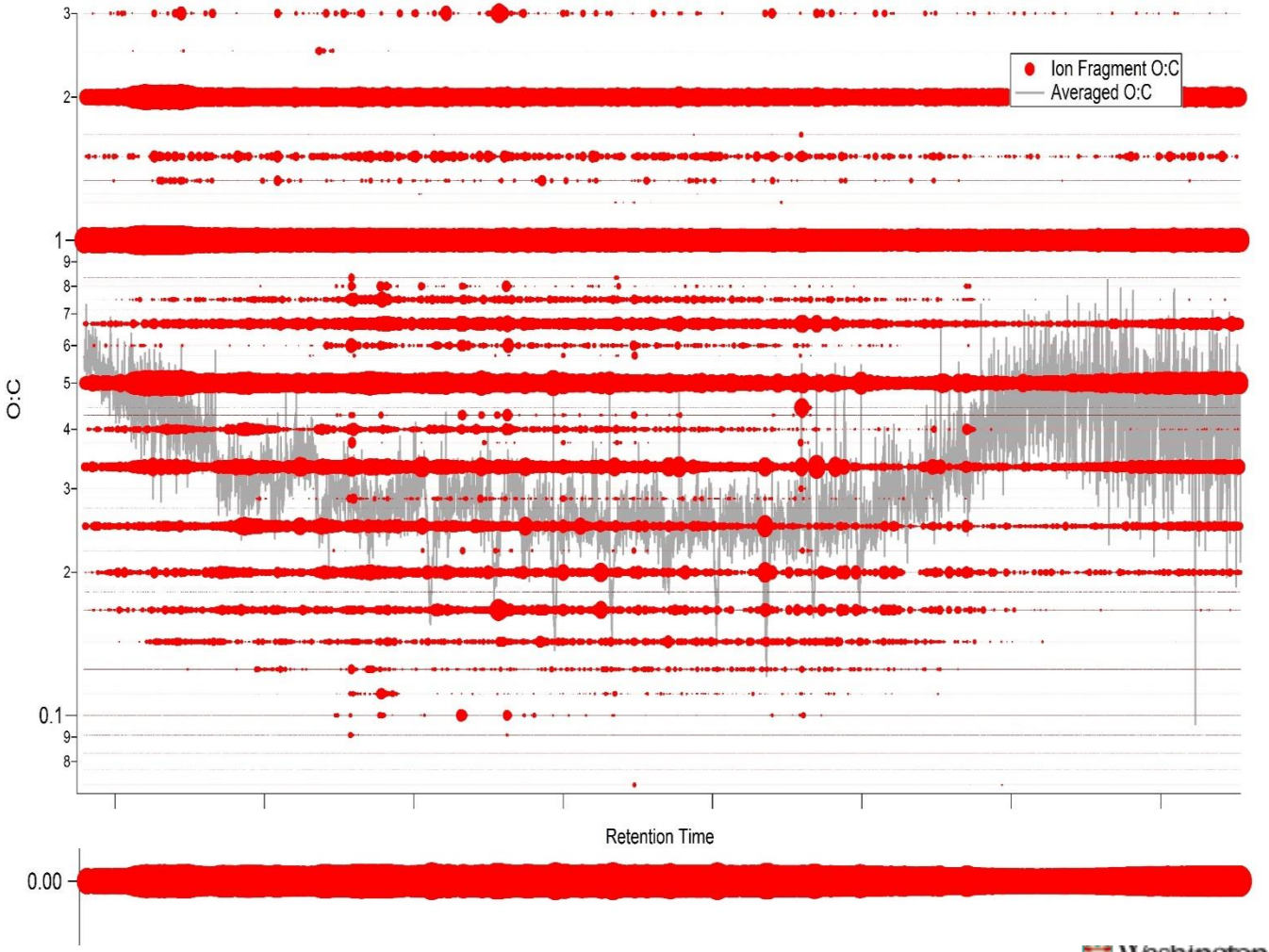
O:C (Ion Fragments) versus Retention Time

Collection Time: 8:15 – 8:45am



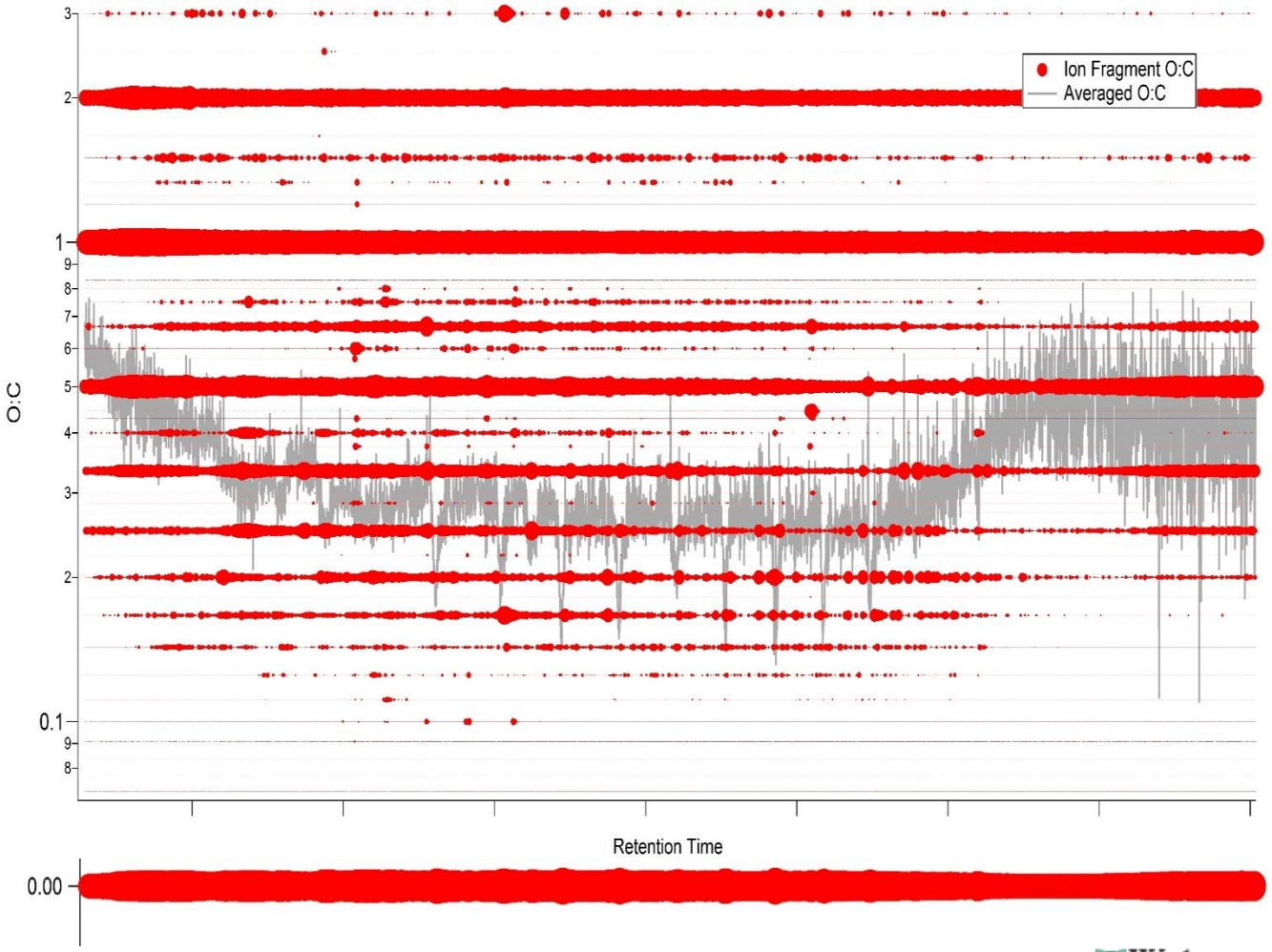
O:C (Ion Fragments) versus Retention Time

Collection Time: 9:45 – 10:15am



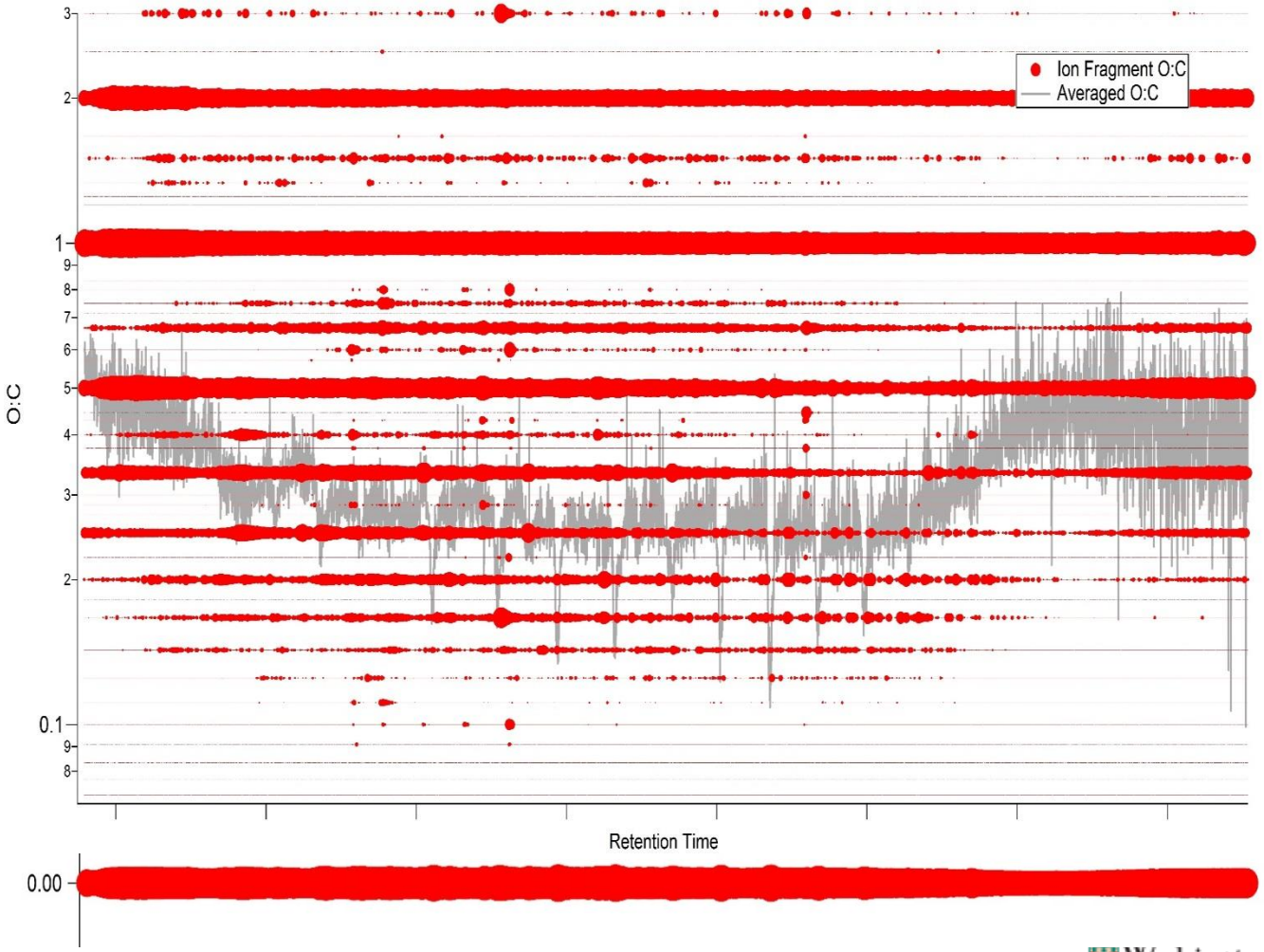
O:C (Ion Fragments) versus Retention Time

Collection Time: 10:30 – 11:00am



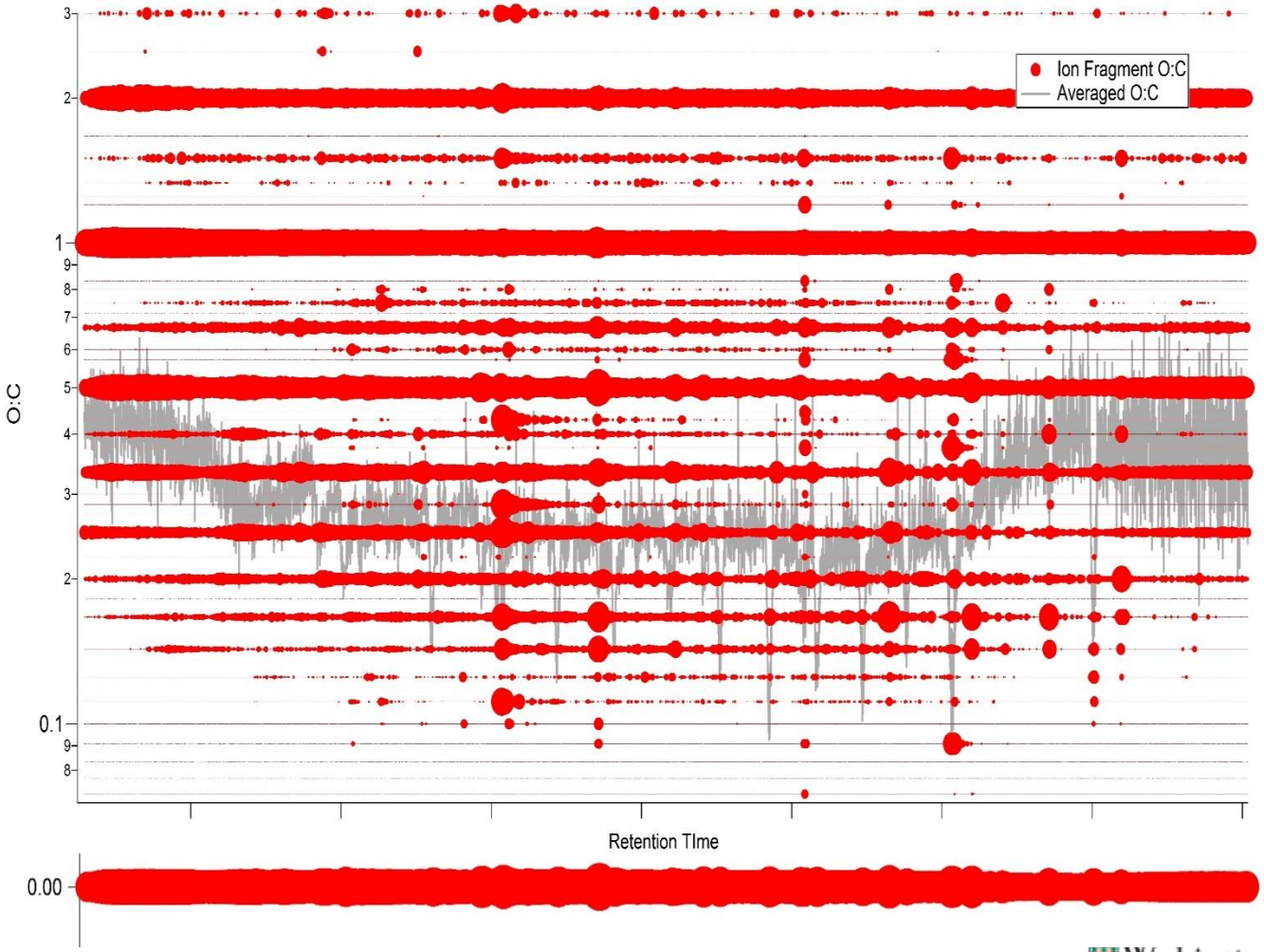
O:C (Ion Fragments) versus Retention Time

Collection Time: 11:15 – 11:45am



O:C (Ion Fragments) versus Retention Time

Collection Time: 12:00 - 12:30pm



Conclusions

- Deployed new instrument offering unique way of measuring organic aerosol
- PMF Factors have good correlation with AMS PMF Factors offering additional chemical identification

Future Work

- Laboratory study of standards and PAM oxidation
- Identify and integrate compounds and obtain time series
- Refine PMF and look for correlations with other measurements