



北京大学环境科学与工程学院
College of Environmental Sciences and Engineering

“Aerodyne AMS/CIMS 北大研讨会”会议通知

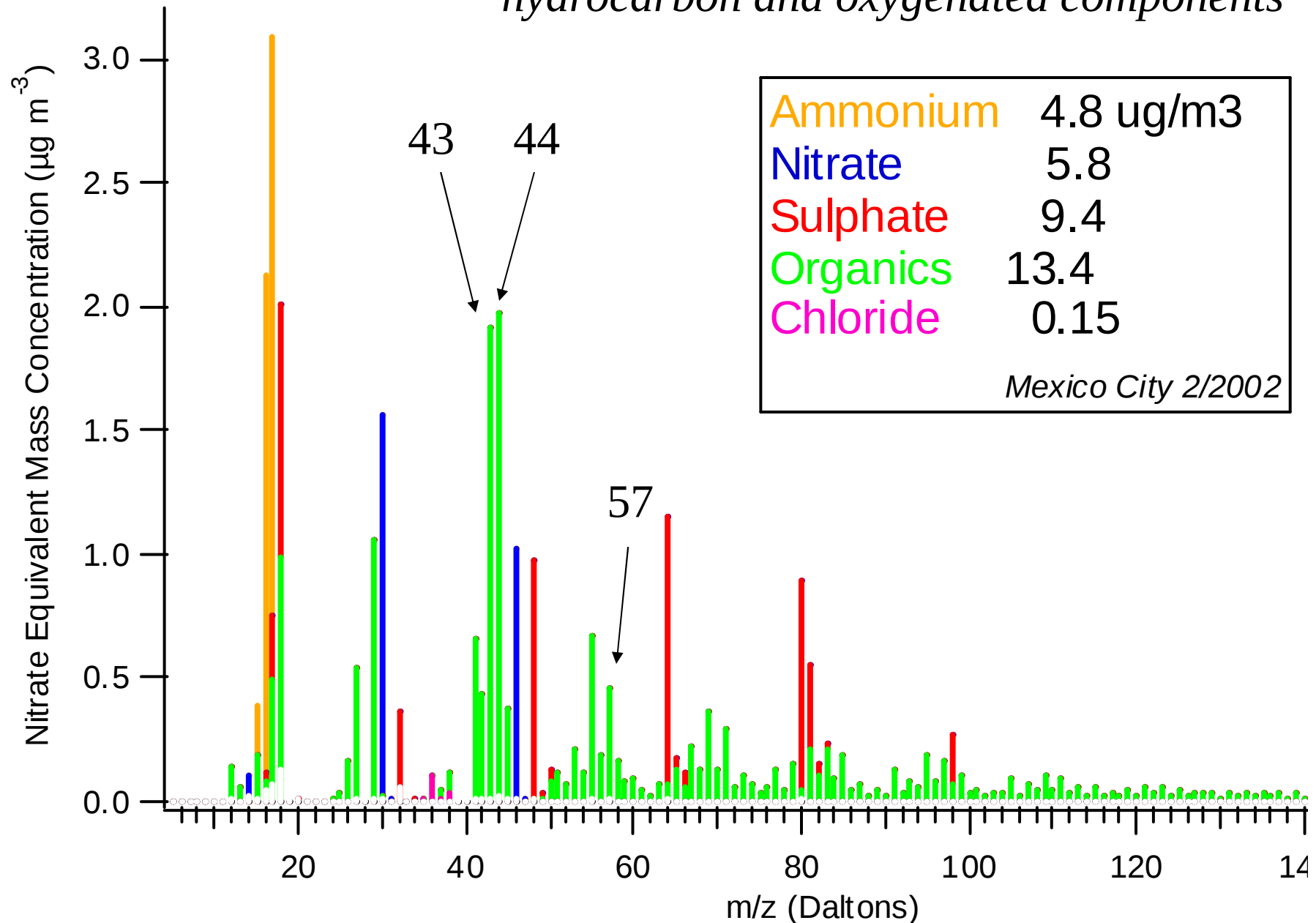
Aerodyne AMS/CIMS 北大研讨会由北京大学环境科学与工程学院协助 Aerodyne 主办，将于 2017 年 5 月 8 日至 5 月 12 日在北京举行。在此，我们诚挚邀请各位莅临参加。

***Some thoughts on high resolution
and peak-fitting***

Doug Worsnop

**ARI/PKU AMS/CIMS Users Meeting
Tuesday, 9 May**

*Urban organic aerosol is a mixture of
hydrocarbon and oxygenated components*



MS Signatures for Aerosol Species Identification

color coded to match spectra

Group	Molecule/Species		Ion Fragments	Mass Fragments
Water	H ₂ O	$\xrightarrow{e^-}$	H ₂ O ⁺ , HO ⁺ , O ⁺	18, 17, 16
Ammonium	NH ₃	$\xrightarrow{e^-}$	NH ₃ ⁺ , NH ₂ ⁺ , NH ⁺	17, 16, 15
Nitrate	HNO ₃	$\xrightarrow{e^-}$	HNO ₃ ⁺ , NO ₂ ⁺ , NO ⁺	63, 46, 30
Sulfate	H ₂ SO ₄	$\xrightarrow{e^-}$	H ₂ SO ₄ ⁺ , HSO ₃ ⁺ , SO ₃ ⁺ SO ₂ ⁺ , SO ⁺	98, 81, 80 64, 48
Organic (Oxygenated)	C _n H _m O _y	$\xrightarrow{e^-}$	H ₂ O ⁺ , CO ⁺ , CO ₂ ⁺ H ₃ C ₂ O ⁺ , HCO ₂ ⁺ , C _n H _m ⁺	18, 28, 44 43, 45, ...
Organic (hydrocarbon)	C _n H _m	$\xrightarrow{e^-}$	C _n H _m ⁺	27, 29, 41, 43, 55, 57, 69, 71...

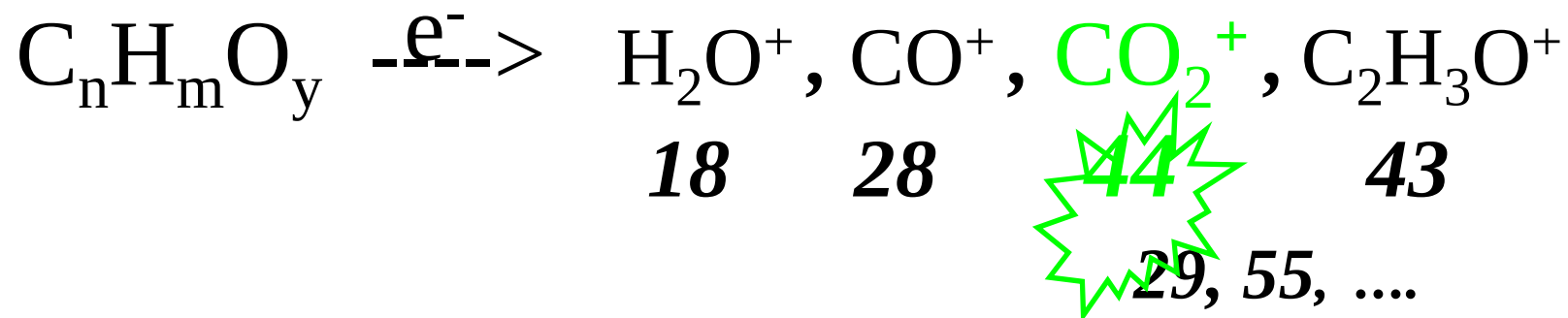
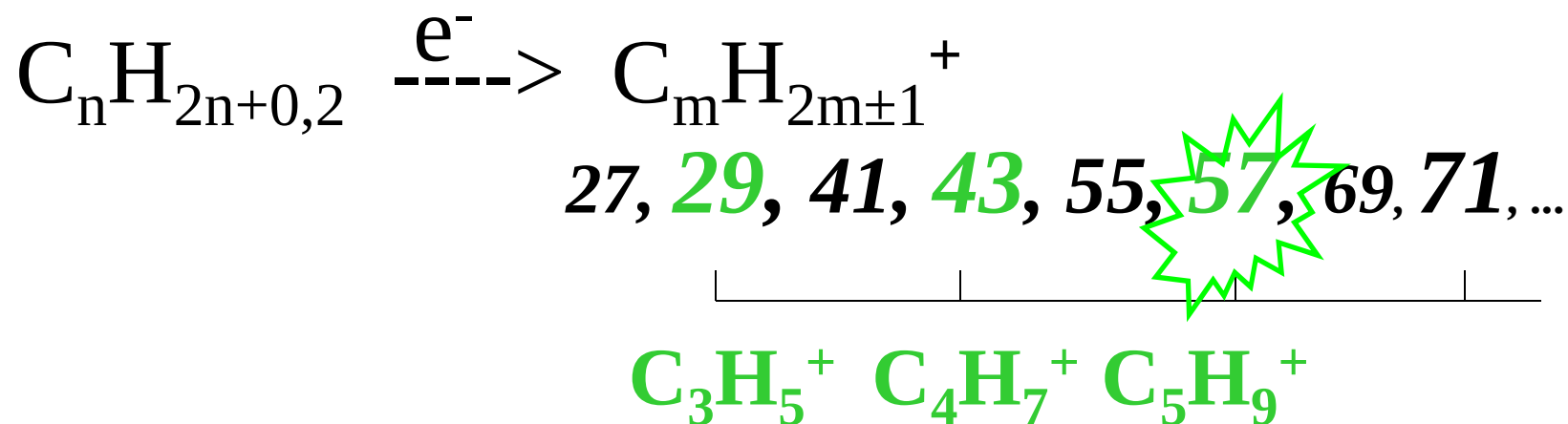
Standard electron impact ionization @ 70 eV

Easy to quantify: ca. NIST MS library

Easy to separate inorganic and organic components

Speciation of organic composition is challenging

Organic Mass Spectra

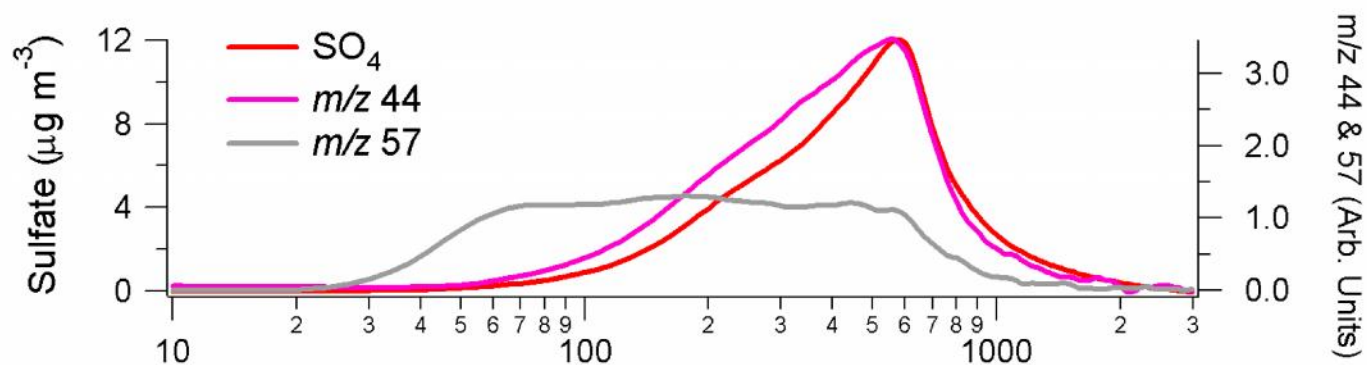
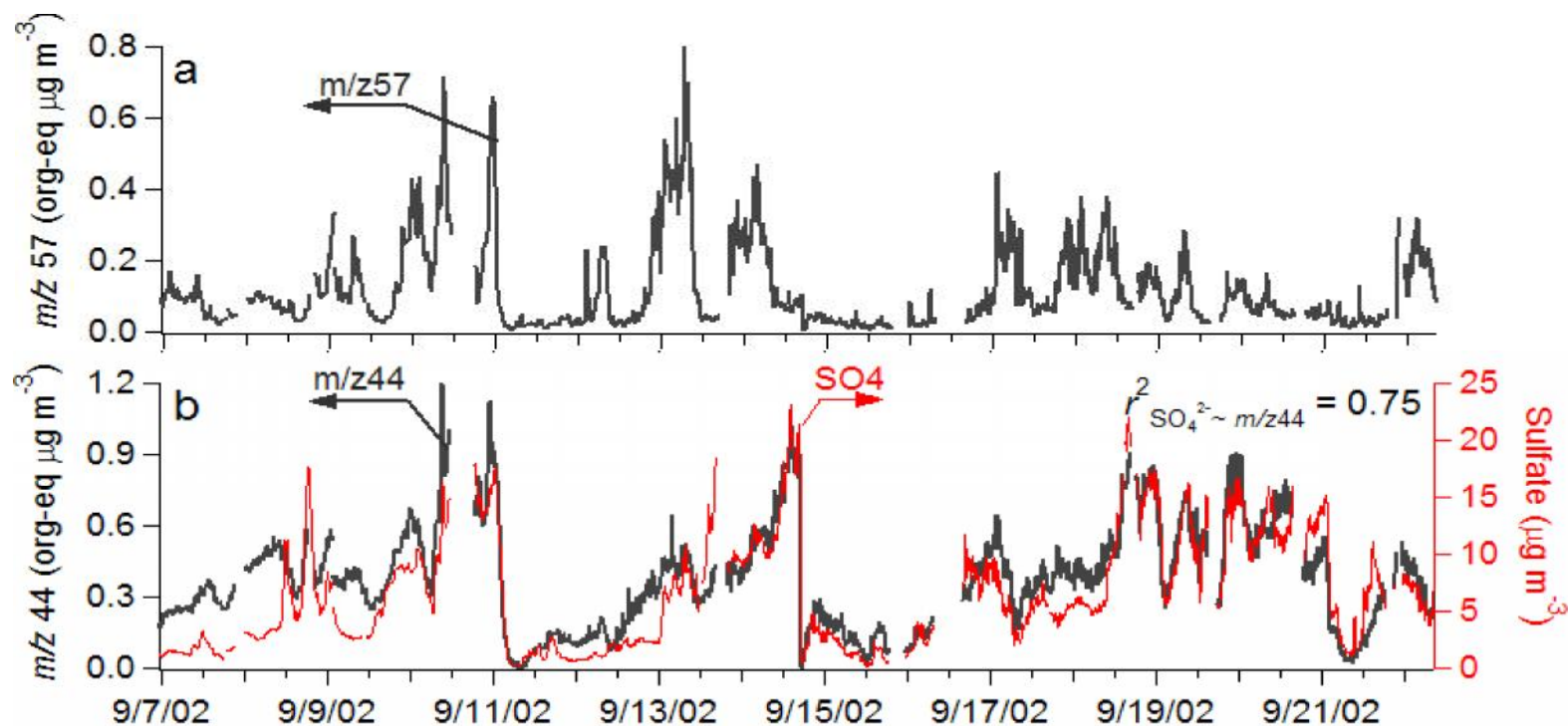


Following flash vaporization at ~600°C

AMS Mass Spectral Tracers

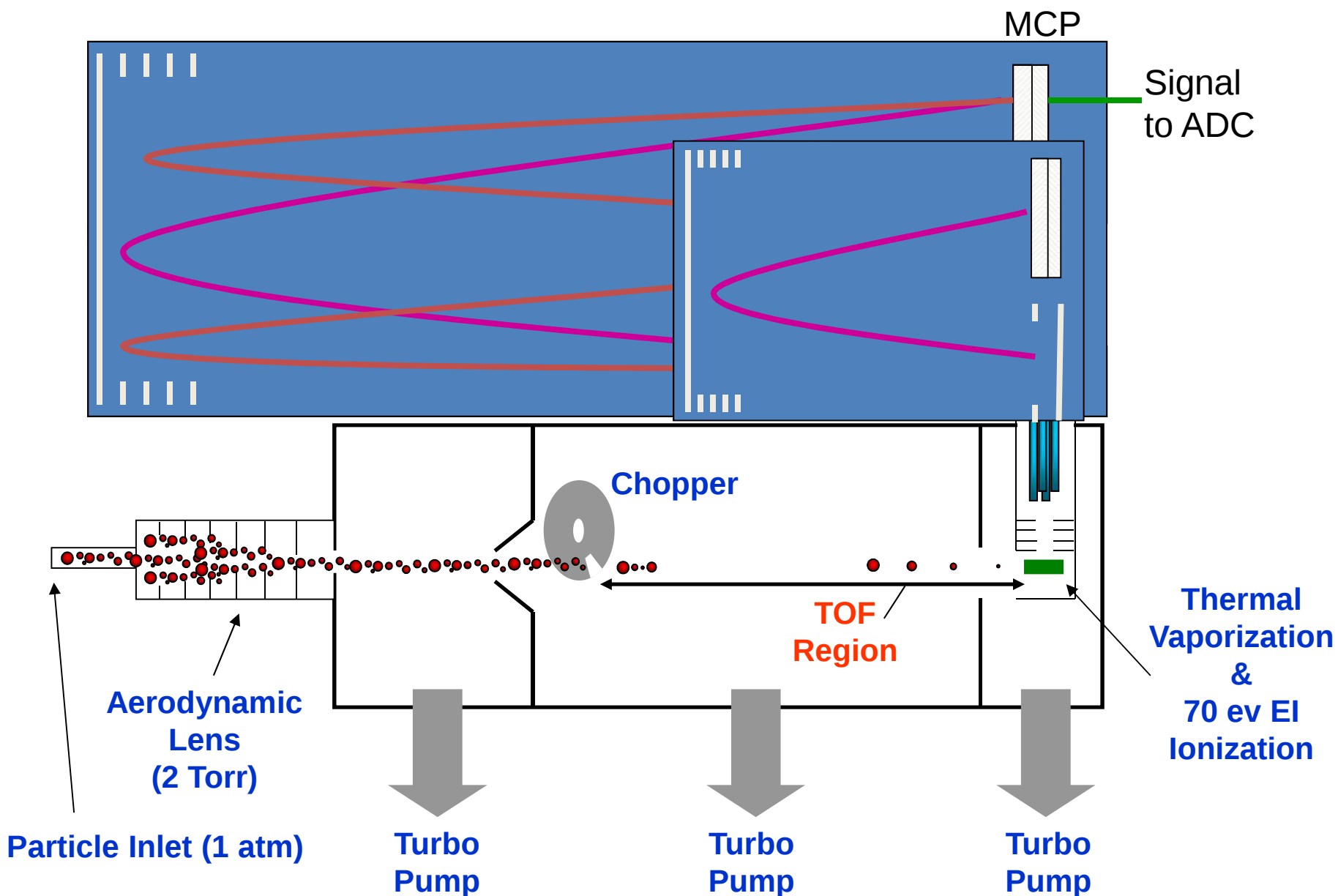
m/z 57 (mostly $C_4H_9^+$): **H**ydrocarbon-like **O**rganic **A**erosol (**HOA**; likely **POA**)

m/z 44 (mostly CO_2^+): **O**xygenated **O**rganic **A**erosol (**OOA**; likely **SOA**)



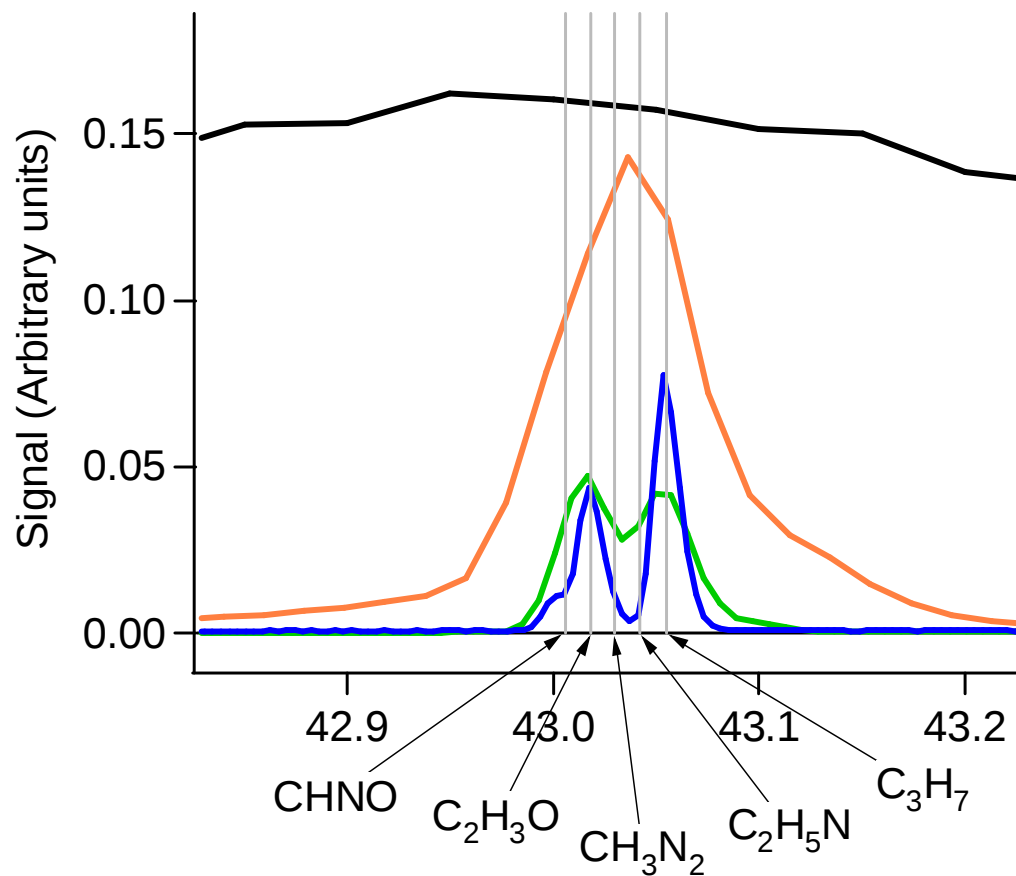
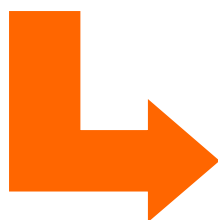
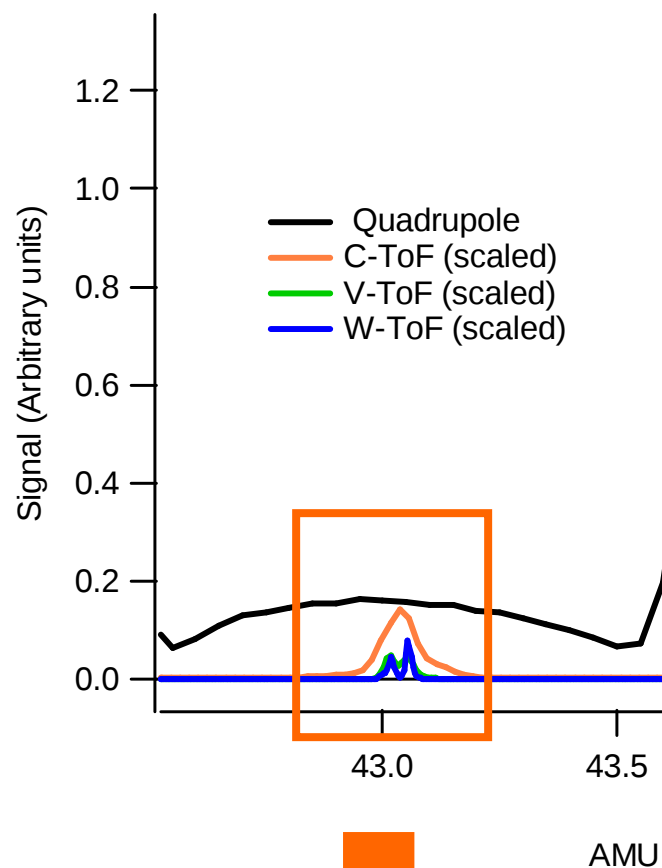
Gas & EC data from
*E. Wittig & R.
Subramanian (CMU)*

New High Resolution ToF-AMS



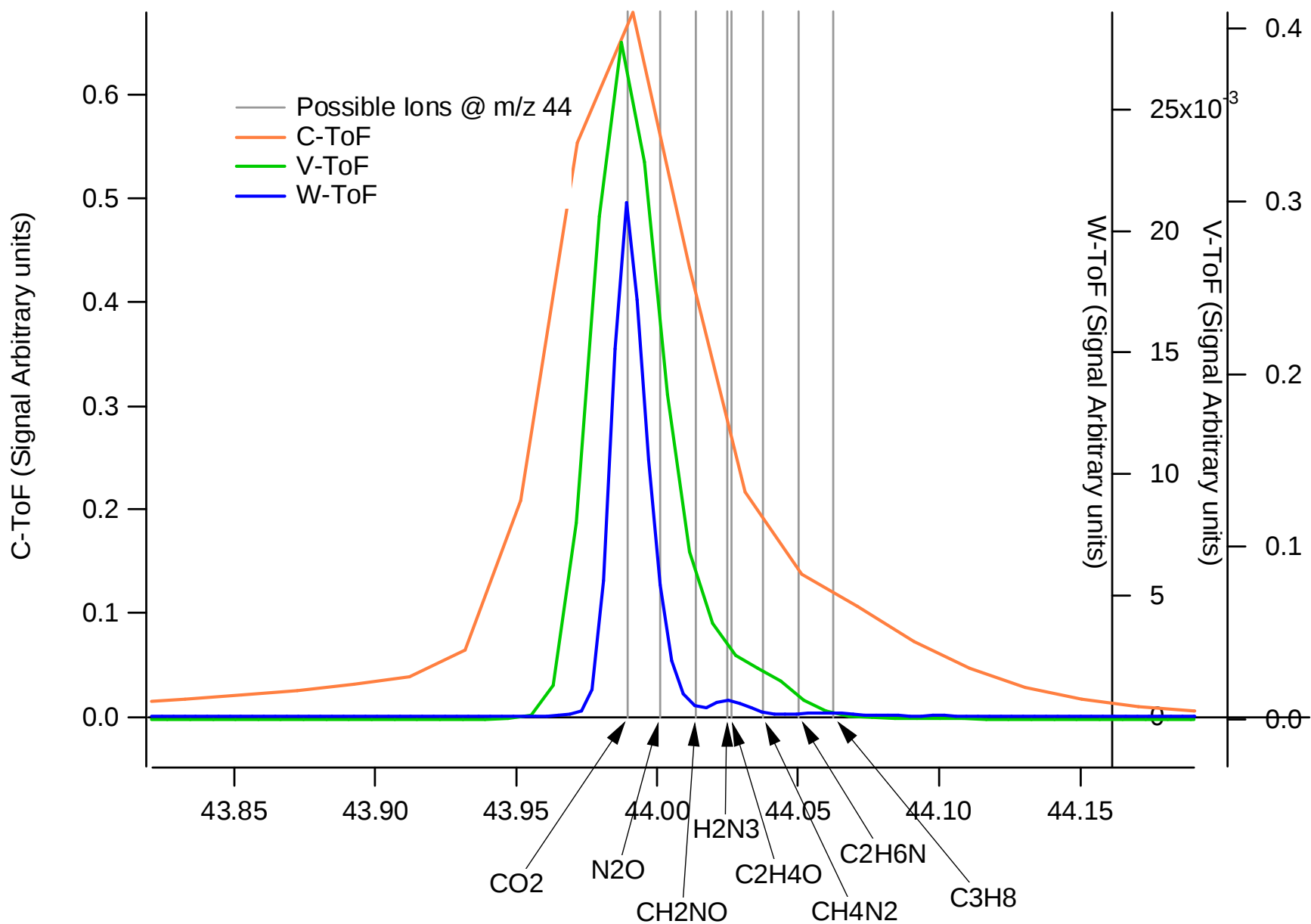
DeCarlo et al., *Anal. Chem.*, in preparation, 2005.

New High Resolution ToF-AMS Spectra



DeCarlo et al., *Anal. Chem.*,
in preparation, 2005.

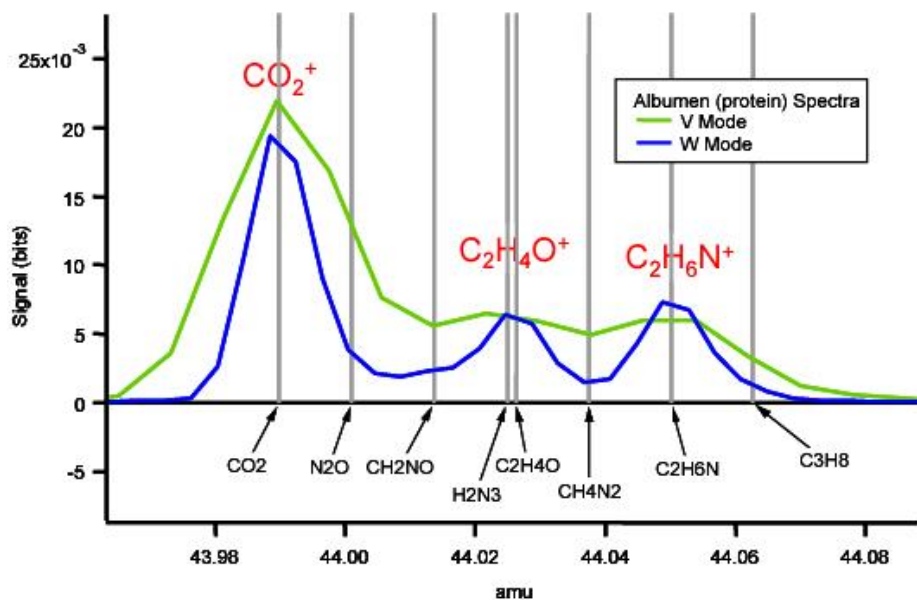
High-Resol. m/z 44 in Ambient Air



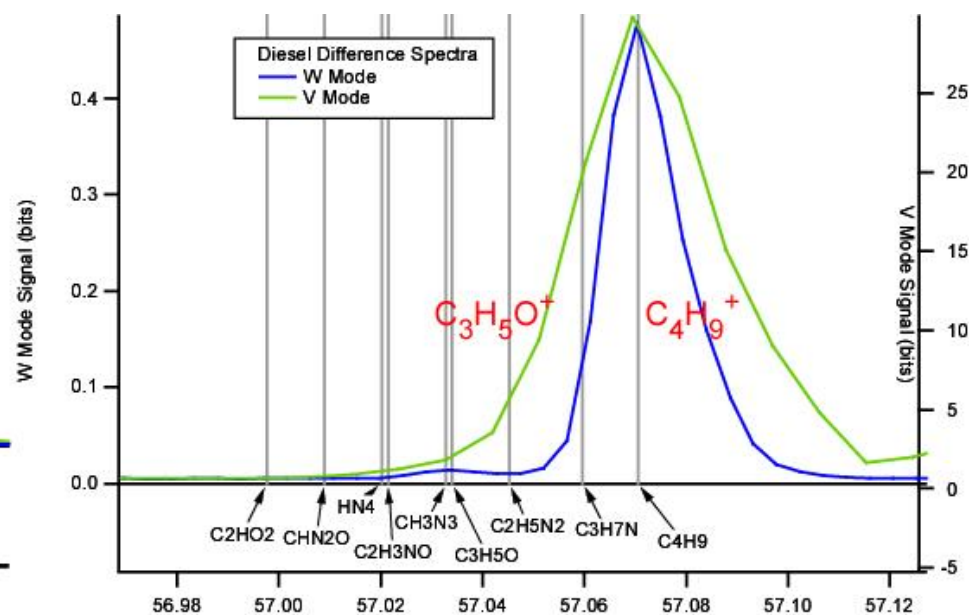
DeCarlo et al., *Anal. Chem.*, in preparation, 2005.

High Resolution MS

Albumen (protein) particles



Diesel Exhaust



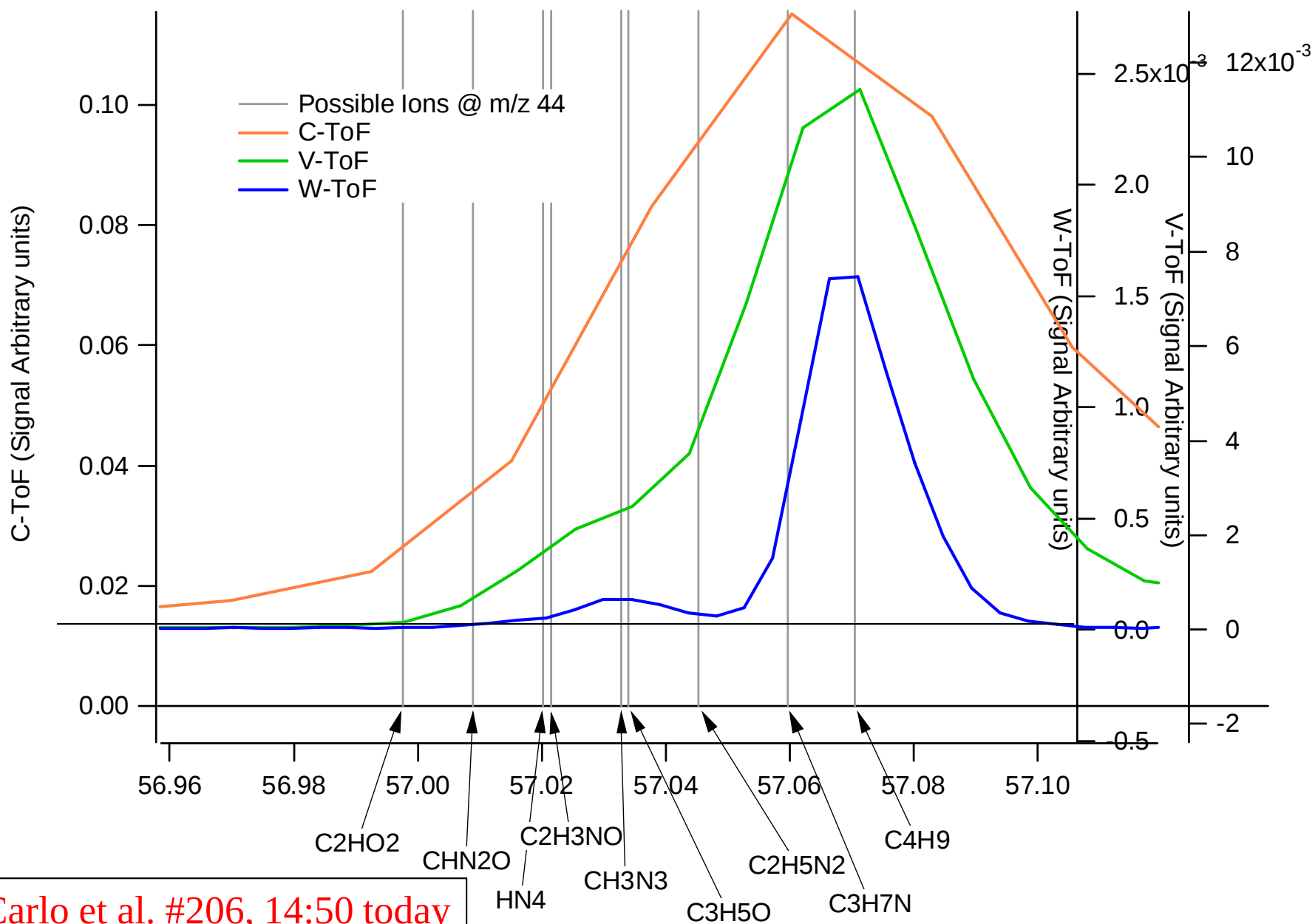
OOA Marker

m/z 44: dominated by CO_2^+

HOA Marker

m/z 57: dominated by C_4H_9^+

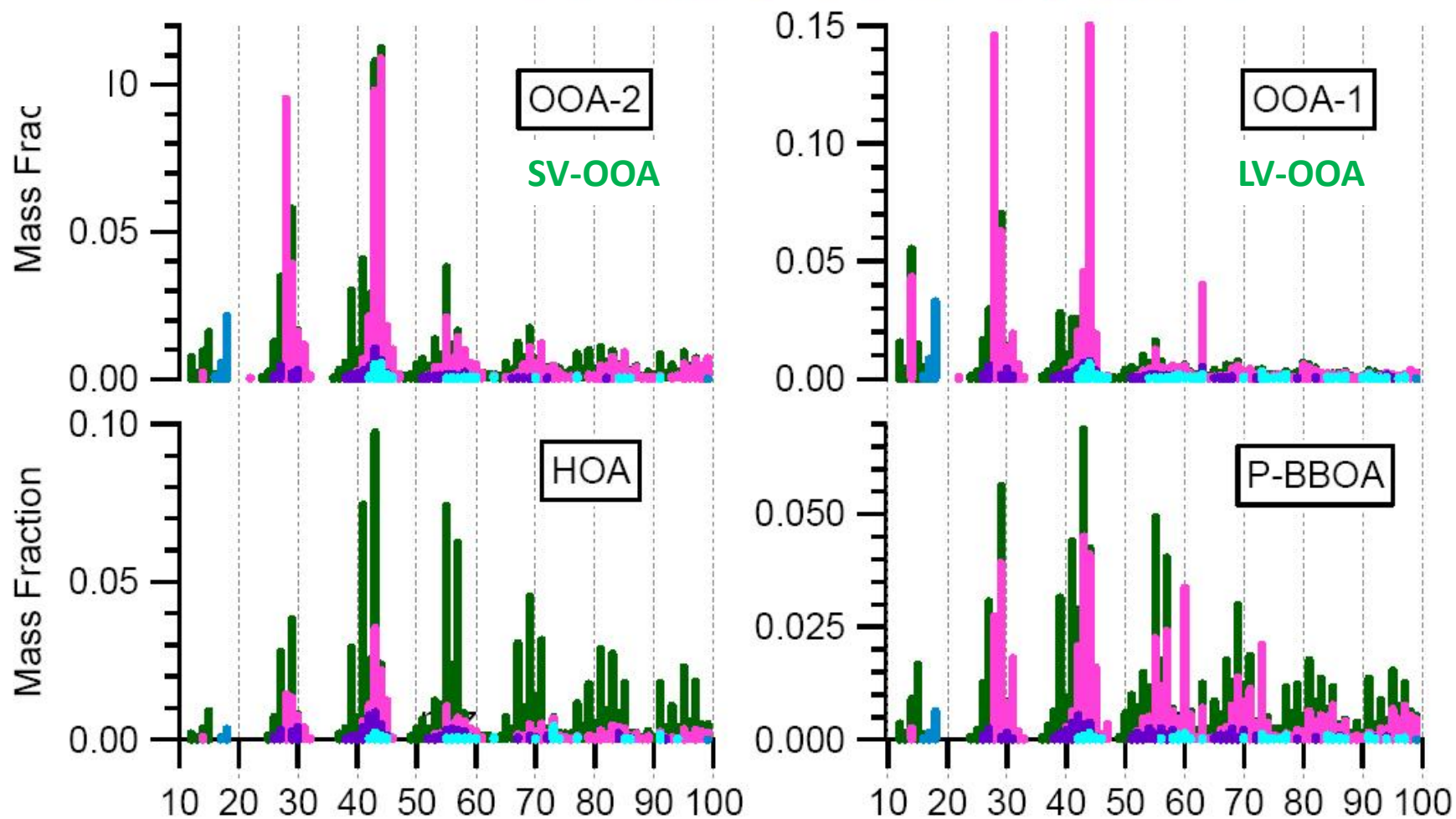
High-Resol. m/z 57 in Ambient Air



DeCarlo et al. #206, 14:50 today

(h)

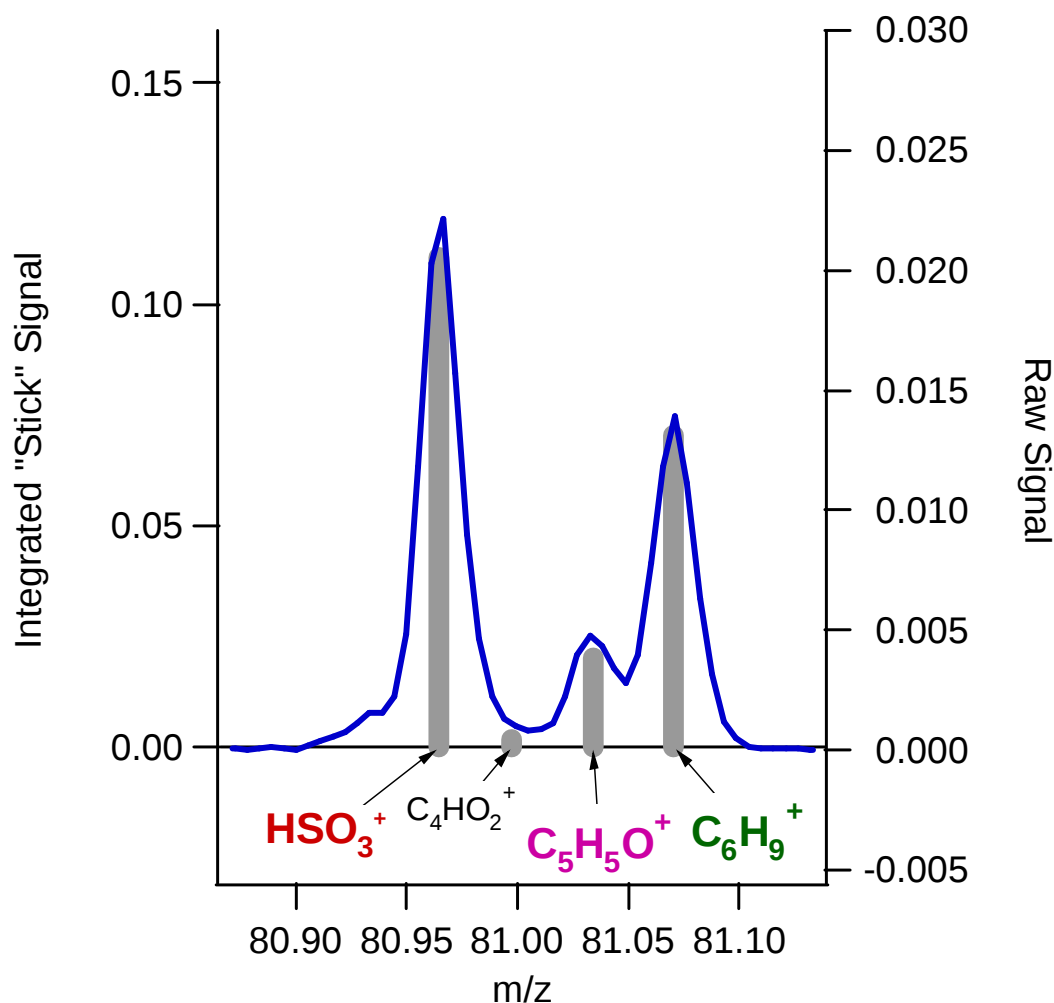
Ion types: C_xH_y , $C_xH_yO_z$, $C_xH_yN_p$, $C_xH_yO_zN_p$, H_xO



Aiken et al, *ES&T*, 2008

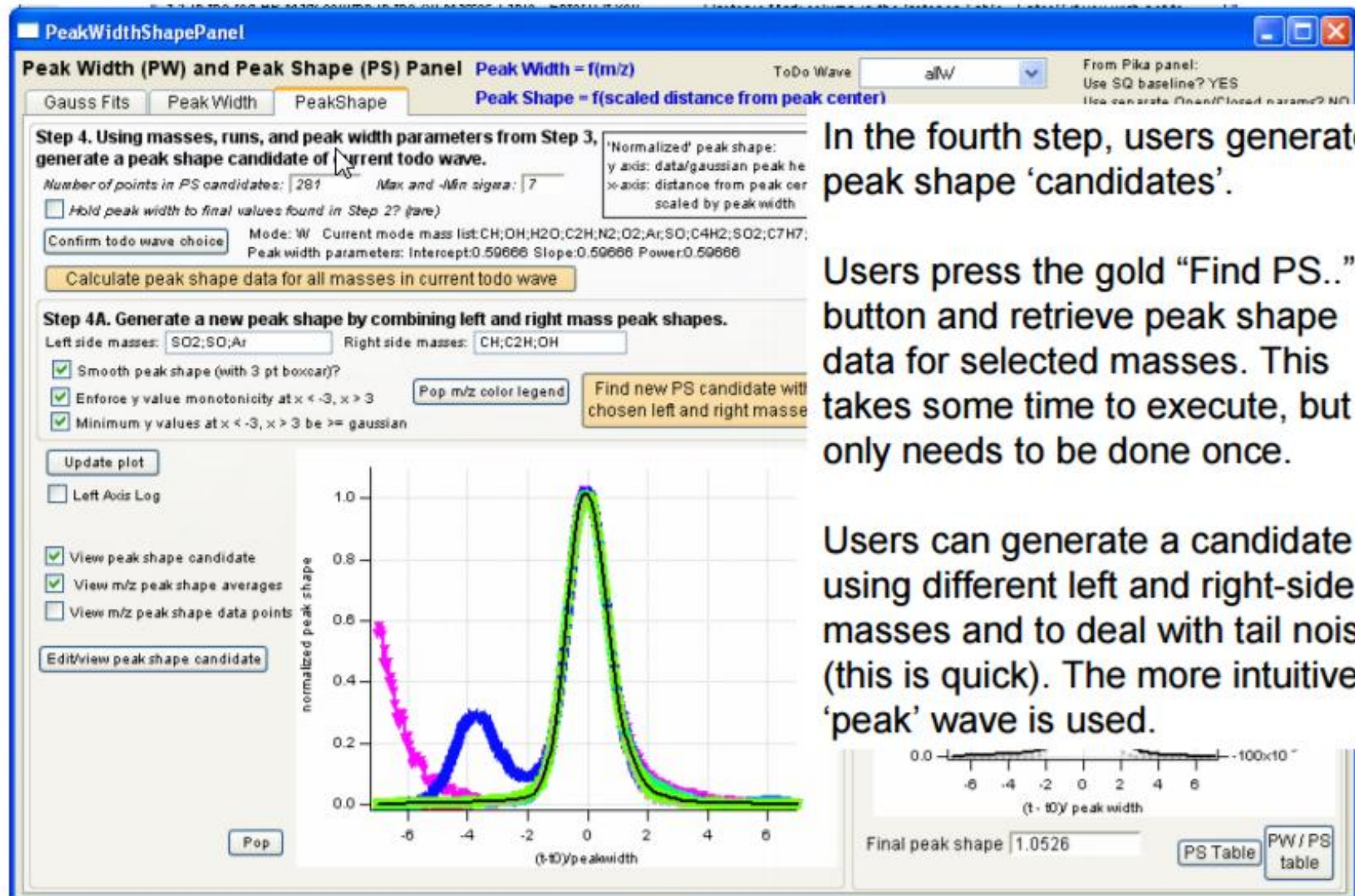
Canagaratna et al, *ACP*, 2015

HR “Sticks”: Quantifying Signal



- m/z 81:
 - inorganic, oxidized, hydrocarbon fragments
- “Custom Peak” fit to expected m/z peaks
- Iterative Process
- Currently for Masses 10-99
- Bar Height equal to total ion area (signal)
- Fitting algorithm still under development

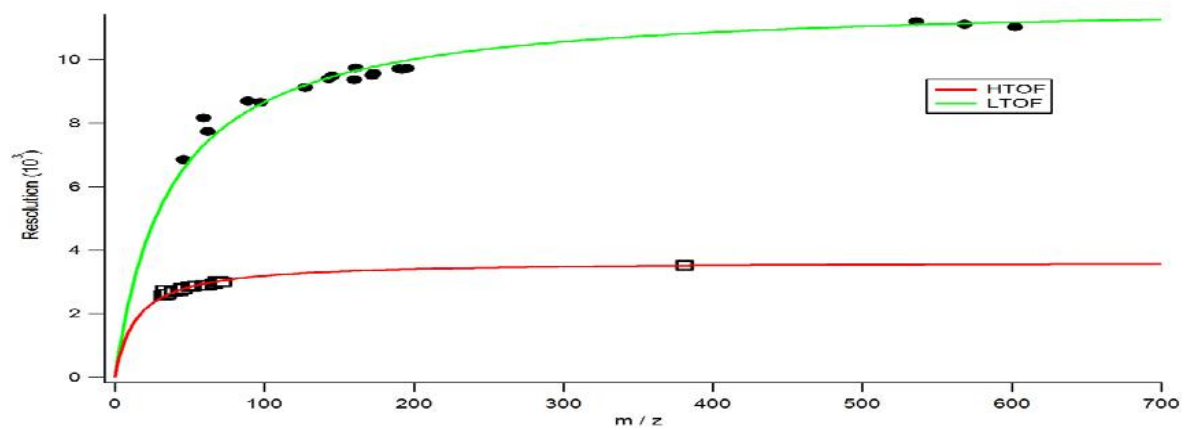
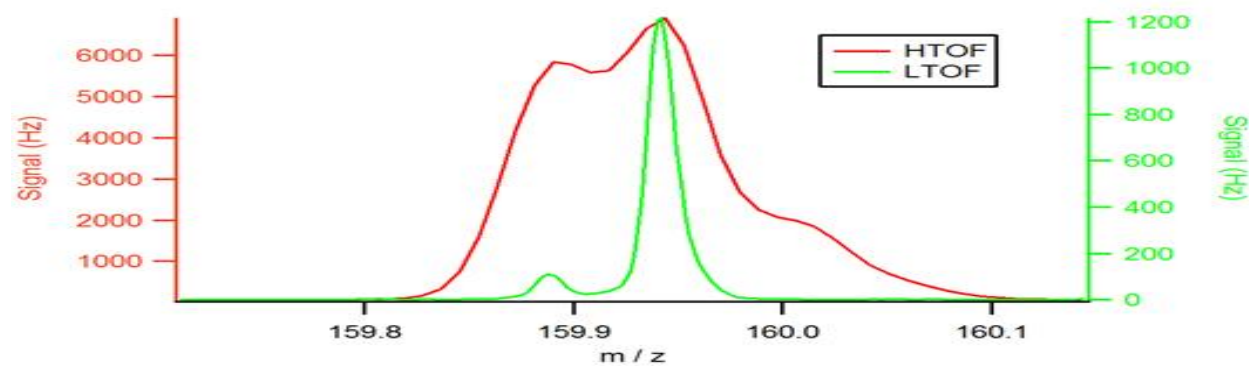
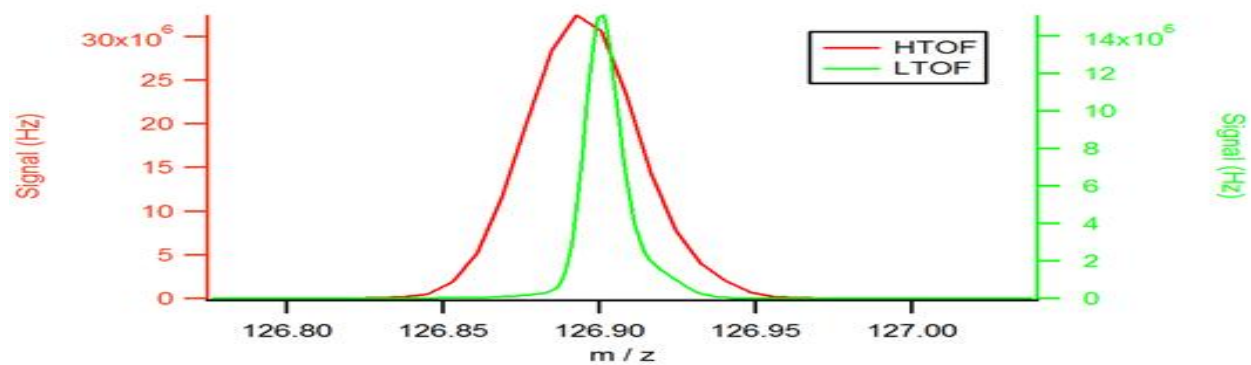
New Peak Width/Shape Panel – peak shape

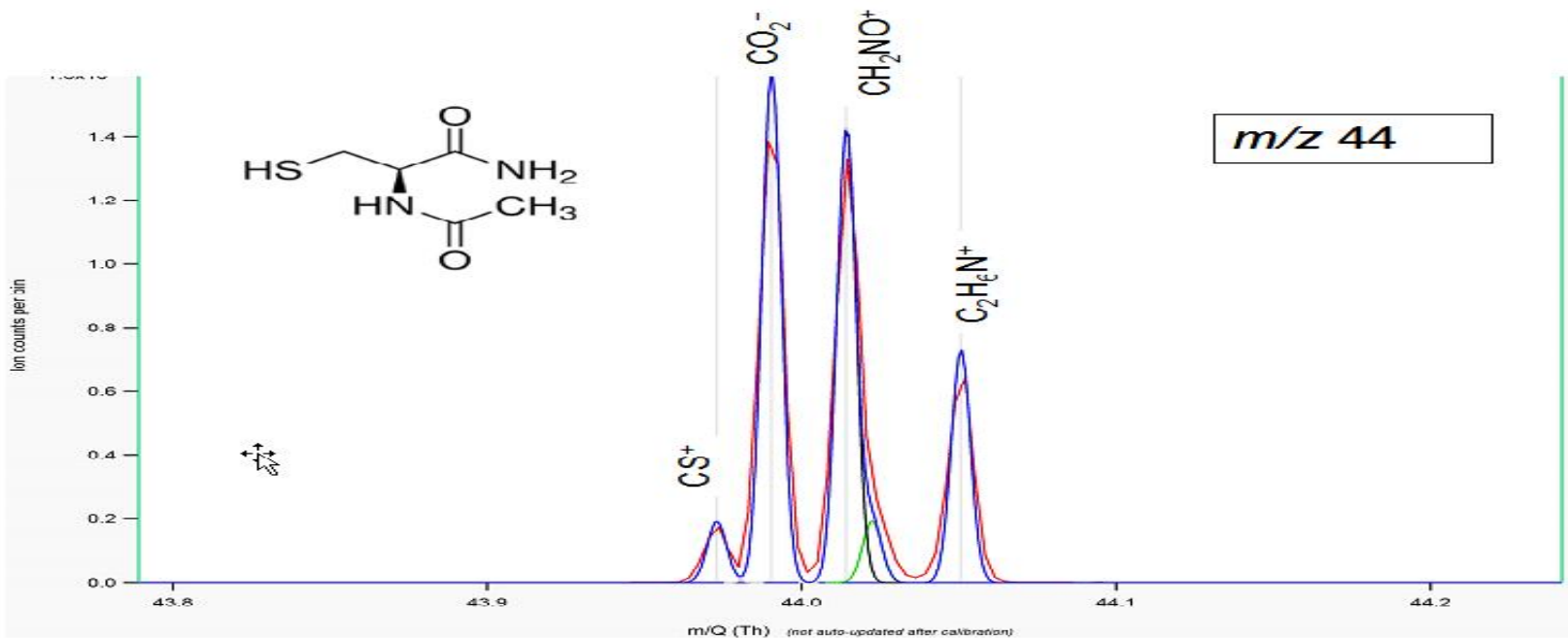


In the fourth step, users generate peak shape 'candidates'.

Users press the gold "Find PS.." button and retrieve peak shape data for selected masses. This takes some time to execute, but only needs to be done once.

Users can generate a candidate using different left and right-side masses and to deal with tail noise (this is quick). The more intuitive 'peak' wave is used.





LToF-AMS (EI)

Resolution > 6000

Red and blue traces – signal and peak shape fitting

[CO_2^+ is mostly background]



Security Studies

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Who Can Keep the Peace? Insurgent Organizational Control of Collective Violence

Alec Worsnop

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