

An Introduction to Orbitraps and Their Capabilities

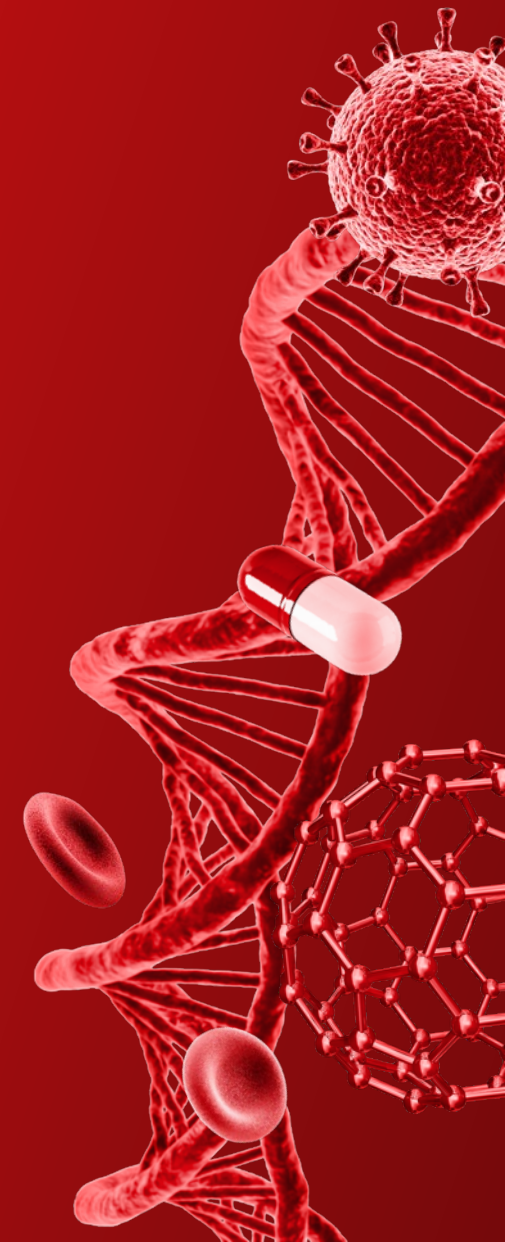
Ken Matuszak

Sr. CMD Product Specialist

 The world leader in serving science

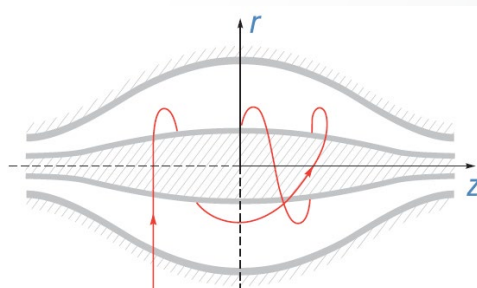


Orbitaps: General principles...

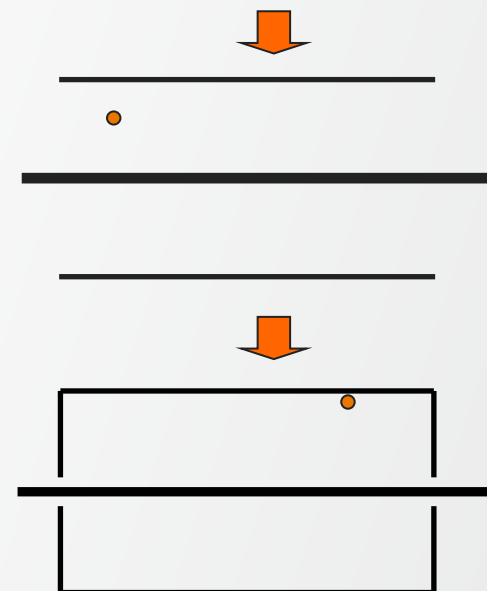


Principle of Trapping in the Orbitrap

- The orbitrap is an ion trap – but there are no RF or magnet fields!
- Moving ions are trapped around an electrode
 - *Electrostatic attraction is compensated by centrifugal force arising from the initial tangential velocity*
- Potential barriers created by end-electrodes confine the ions axially
- One can control the frequencies of oscillations (especially the axial ones) by shaping the electrodes appropriately
- Thus we arrive at ...



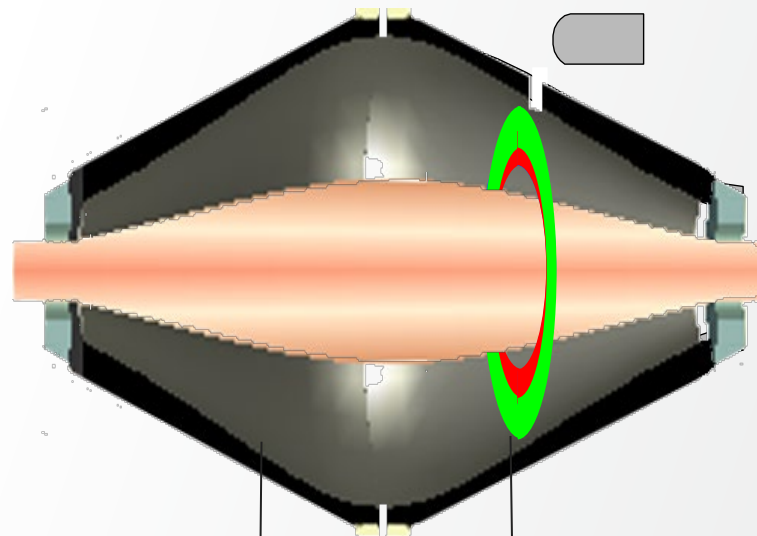
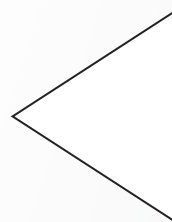
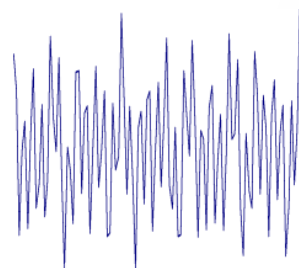
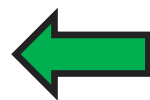
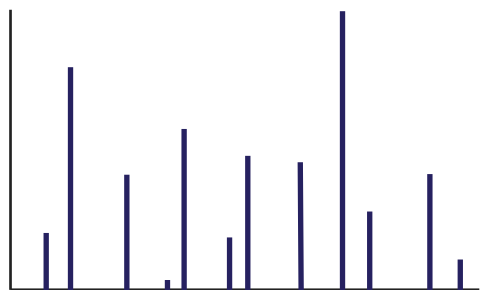
Orbital traps
Kingdon (1923)



Detection of ions in the Orbitrap

- Characteristic frequencies:
 - Frequency of rotation ω_{ϕ} .
 - Frequency of radial oscillations ω_r .
 - Frequency of axial oscillations ω_z .

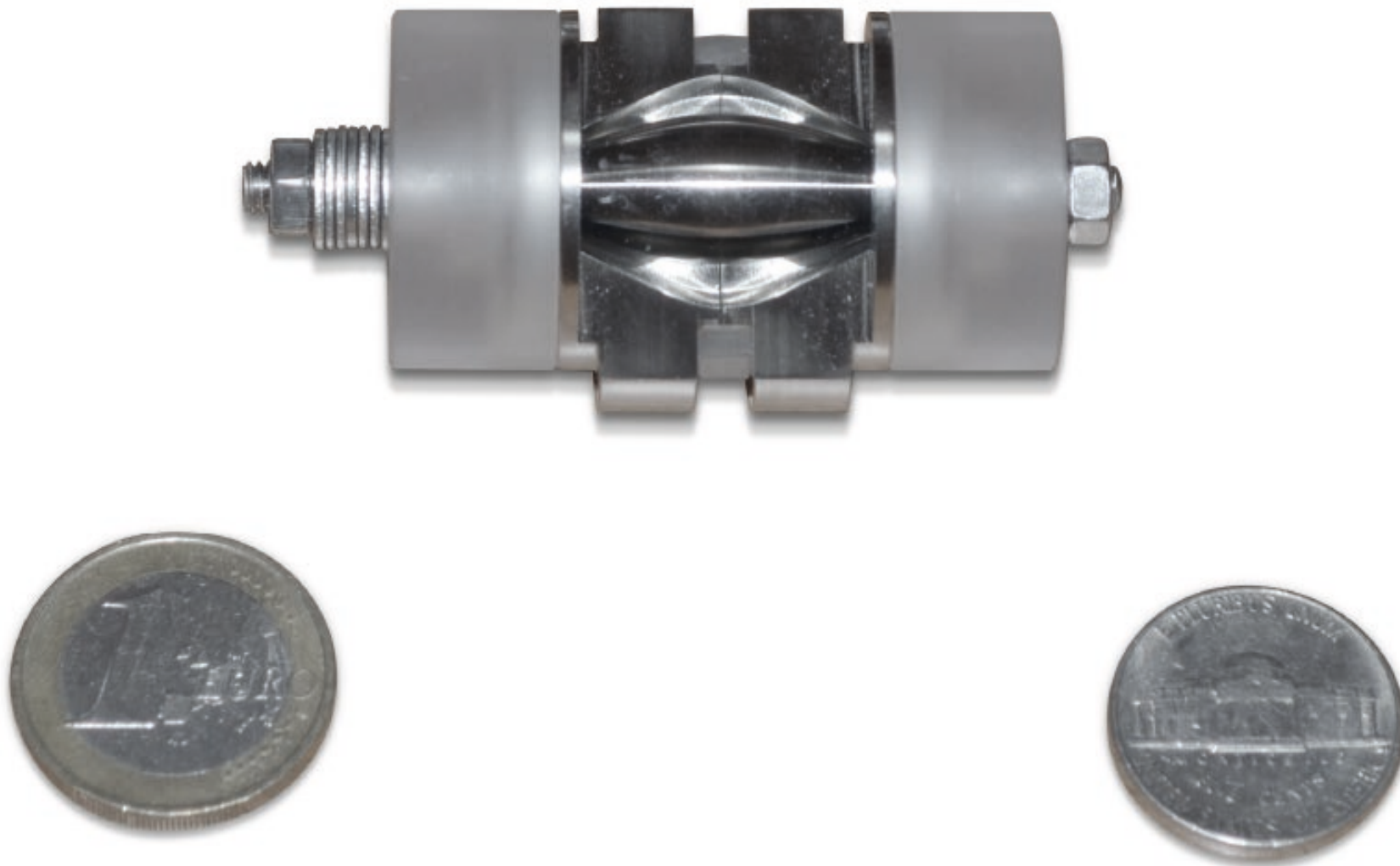
- Multiple ions in the Orbitrap generate a complex signal whose frequencies are determined using a Fourier Transformation.



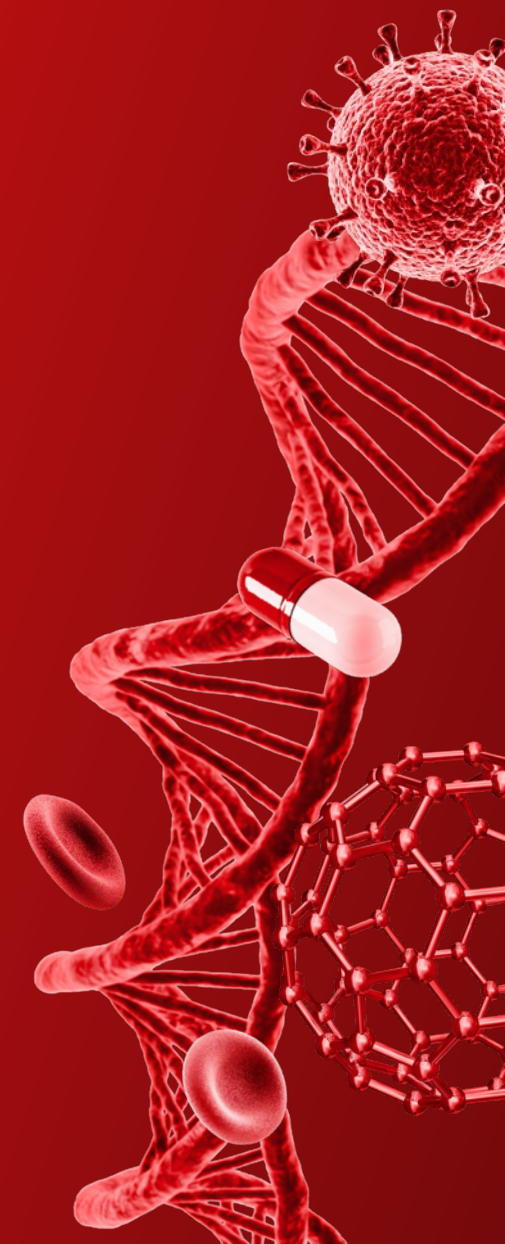
$$\omega_z = \sqrt{\frac{k}{m/q}}$$

ω_z used for mass analysis

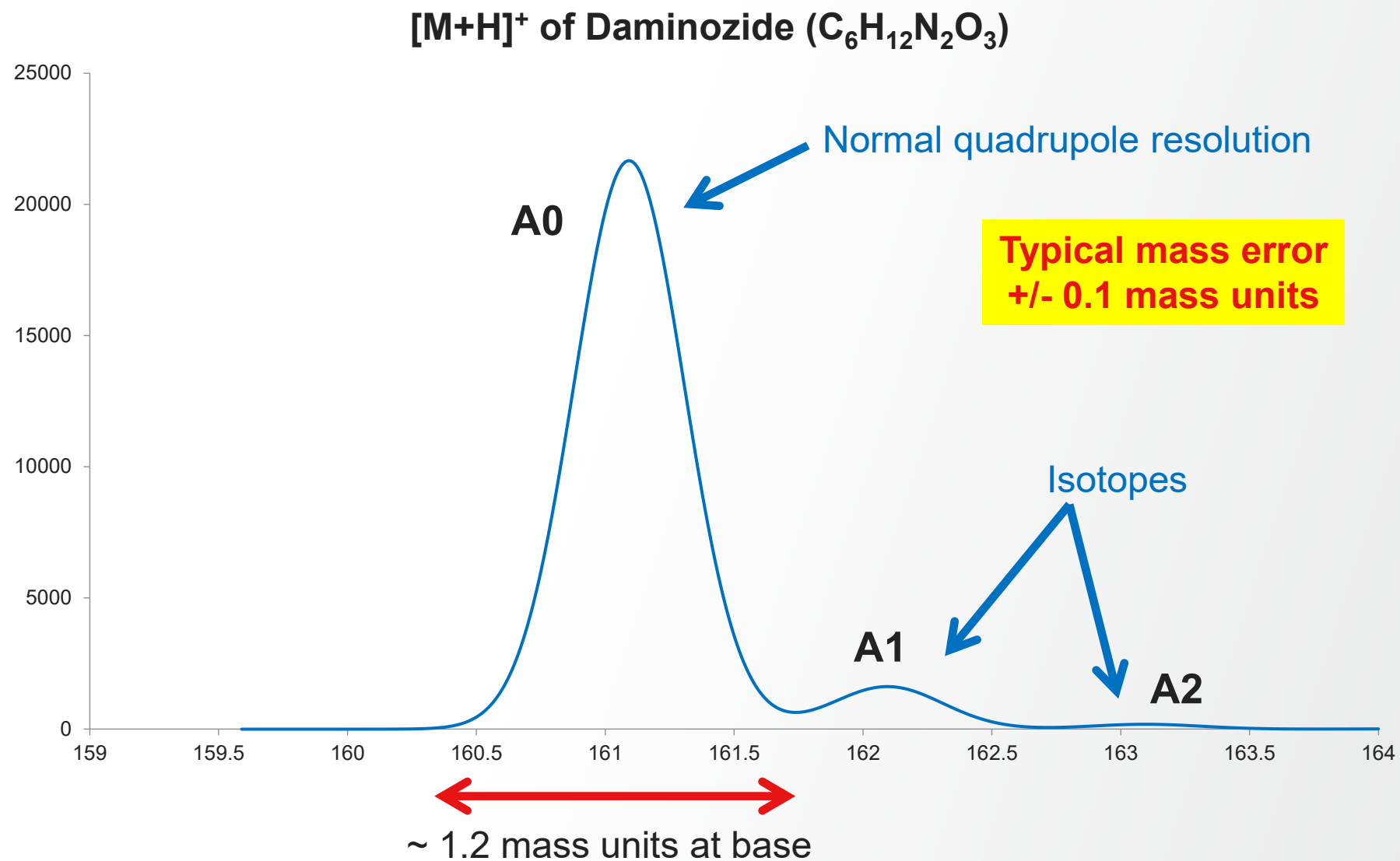
How Big is an Orbitrap?



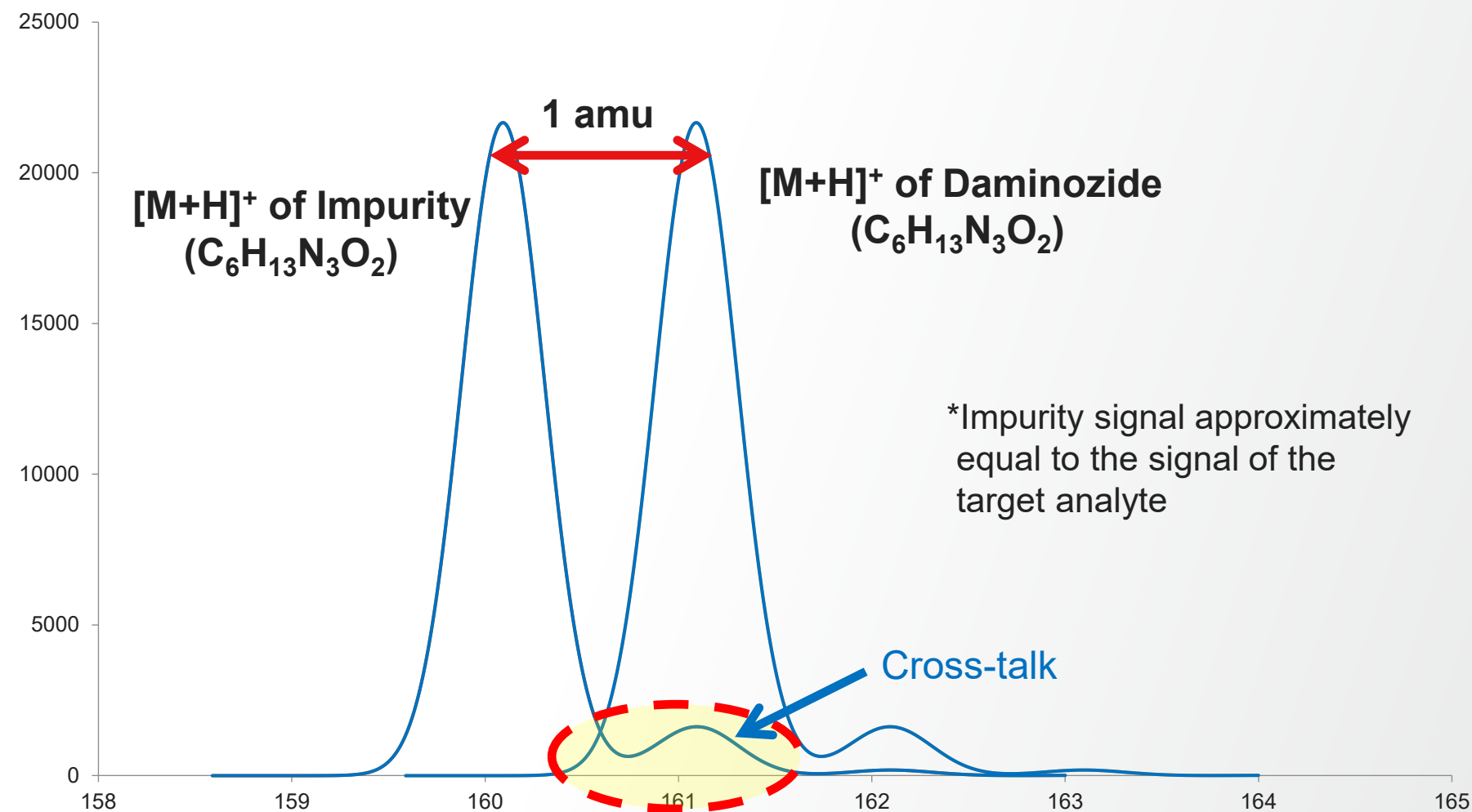
How Different is Orbitrap Resolution from Quadrupole Resolution?



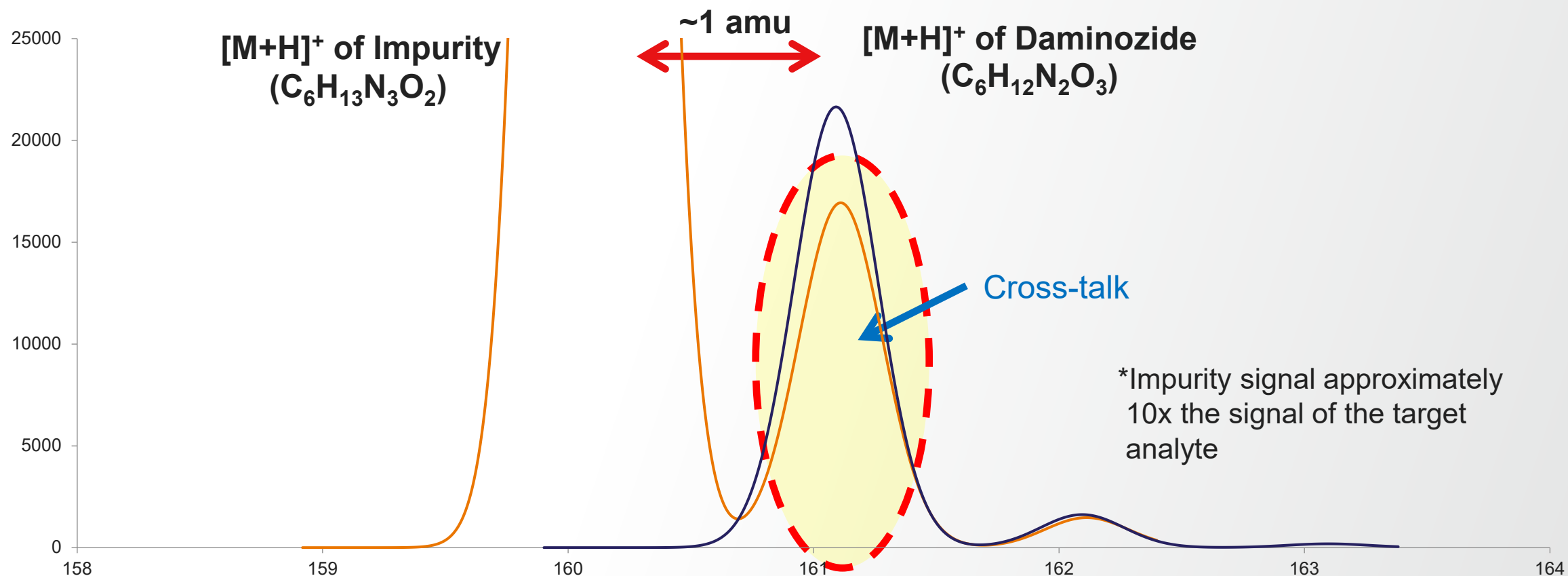
Normal Quadrupole Resolution



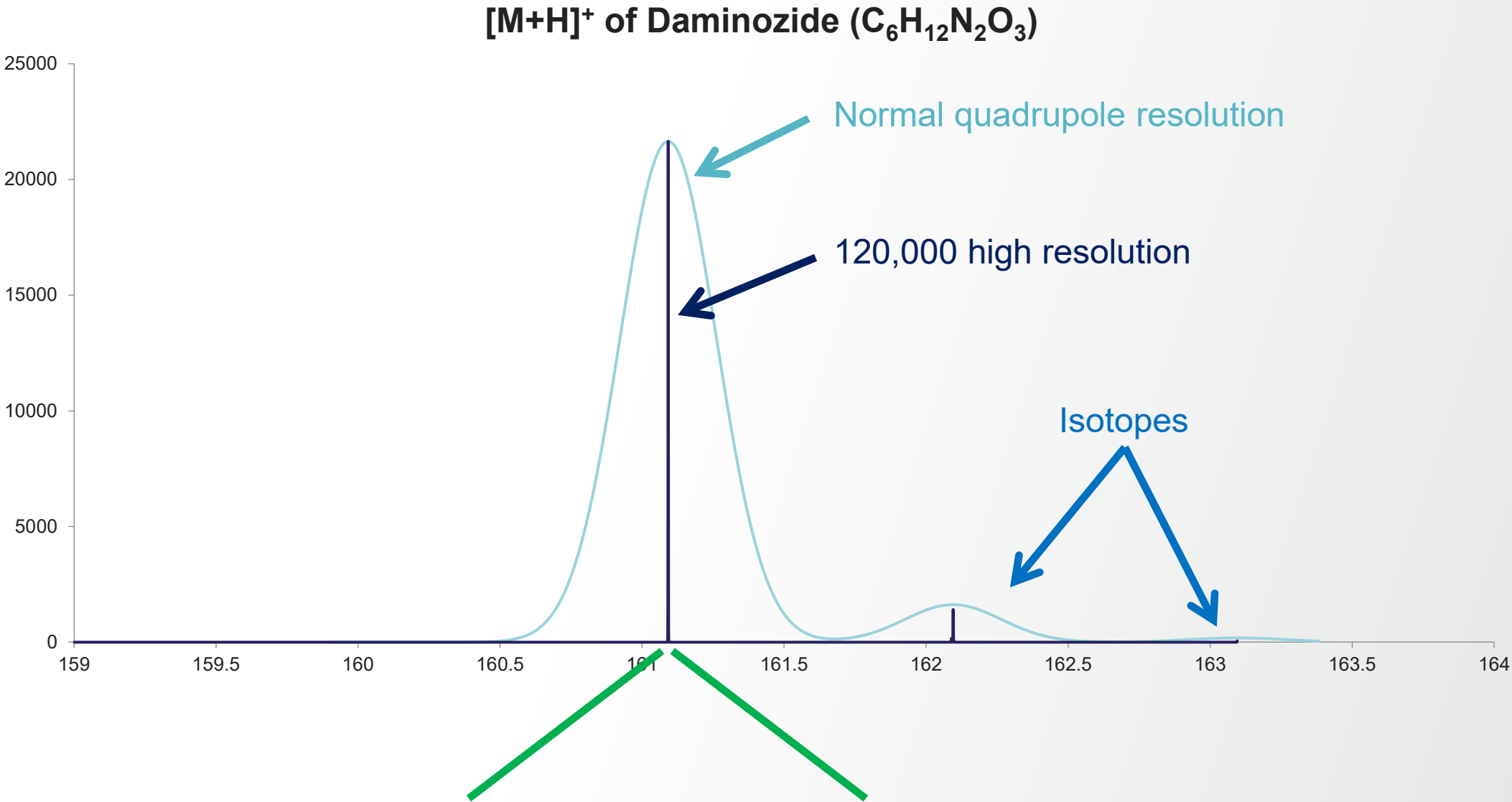
Cross-talk with Quadrupole Resolution



Cross-talk with Quadrupole Resolution

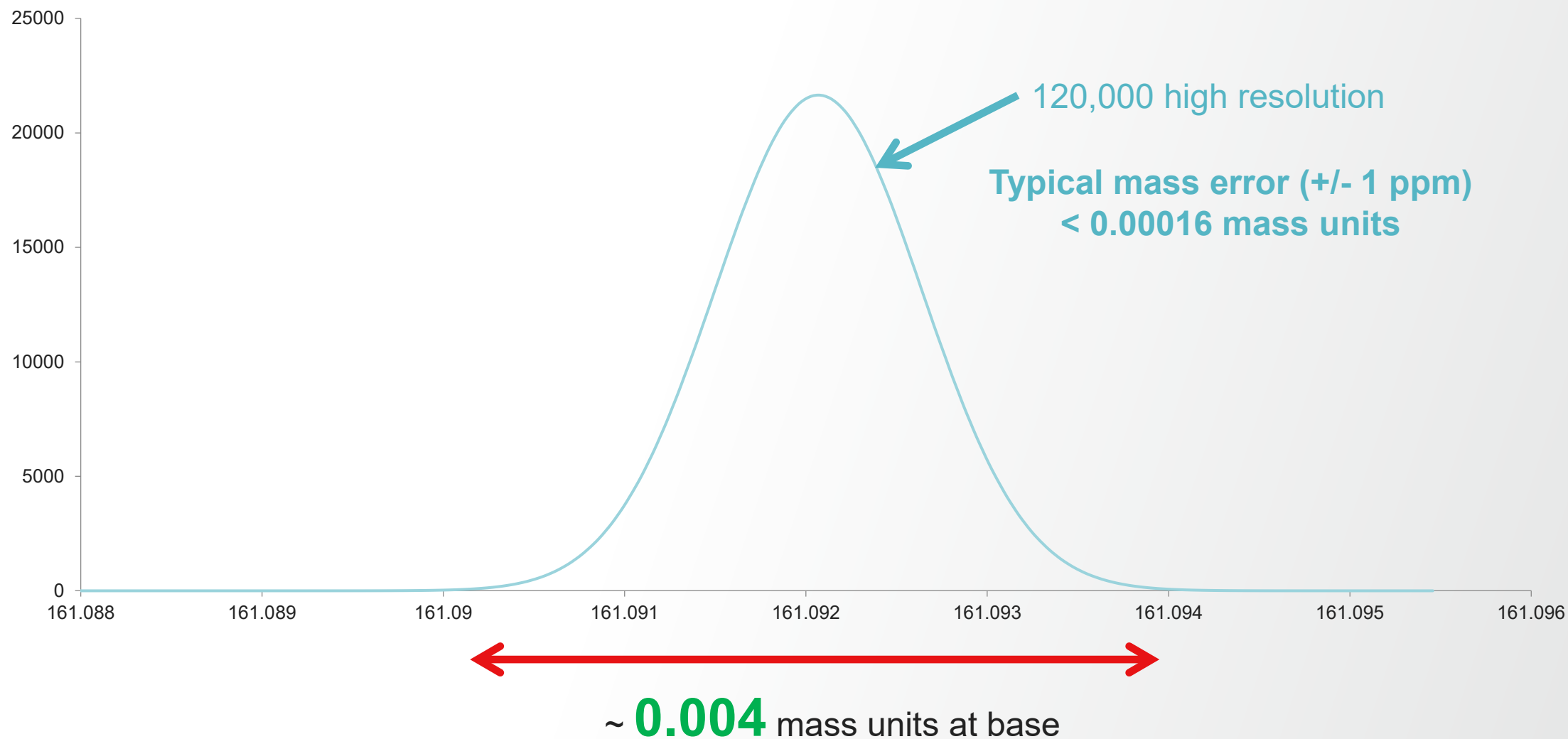


Quad Resolution Compared to High Resolution (120,000)

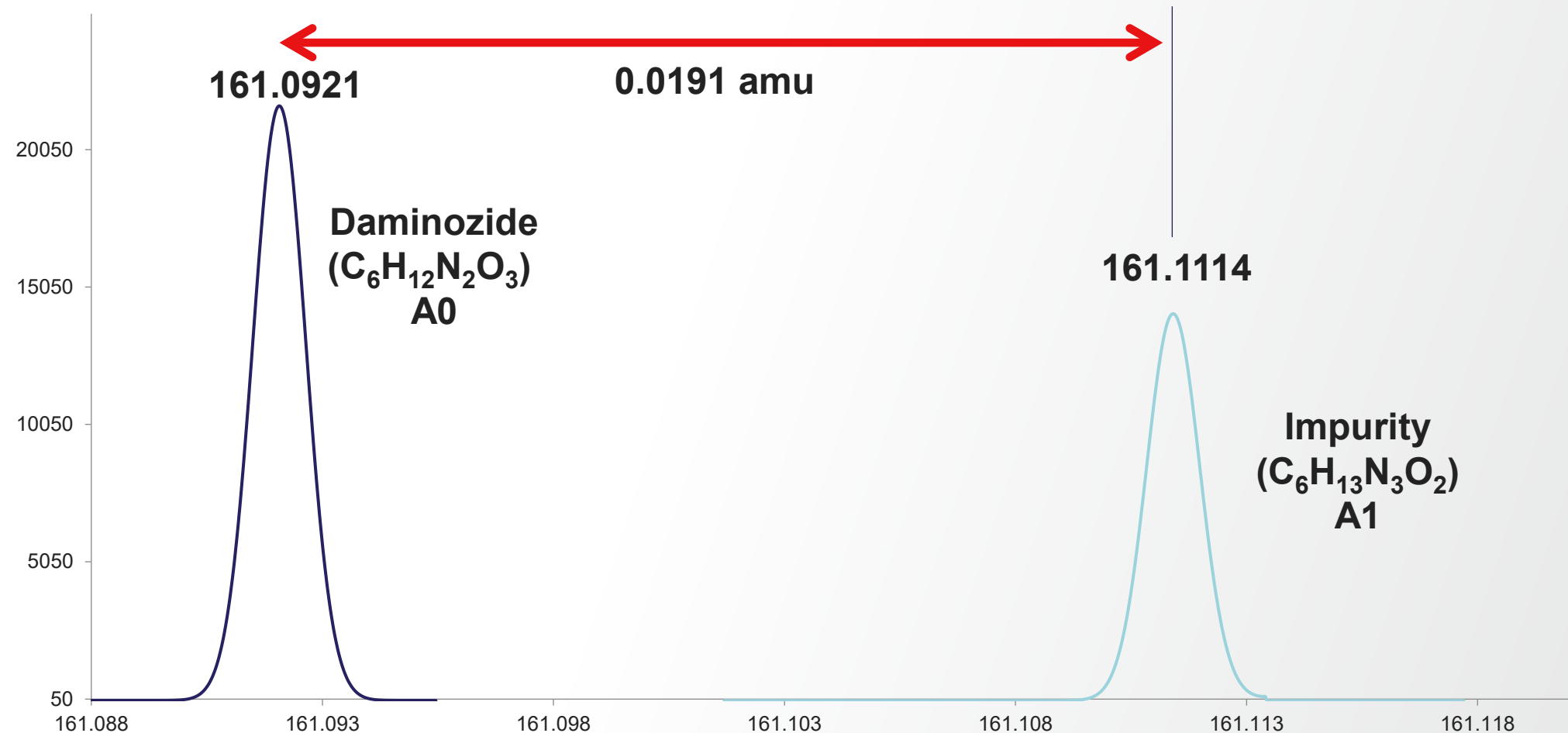


High Resolution (120,000 res)

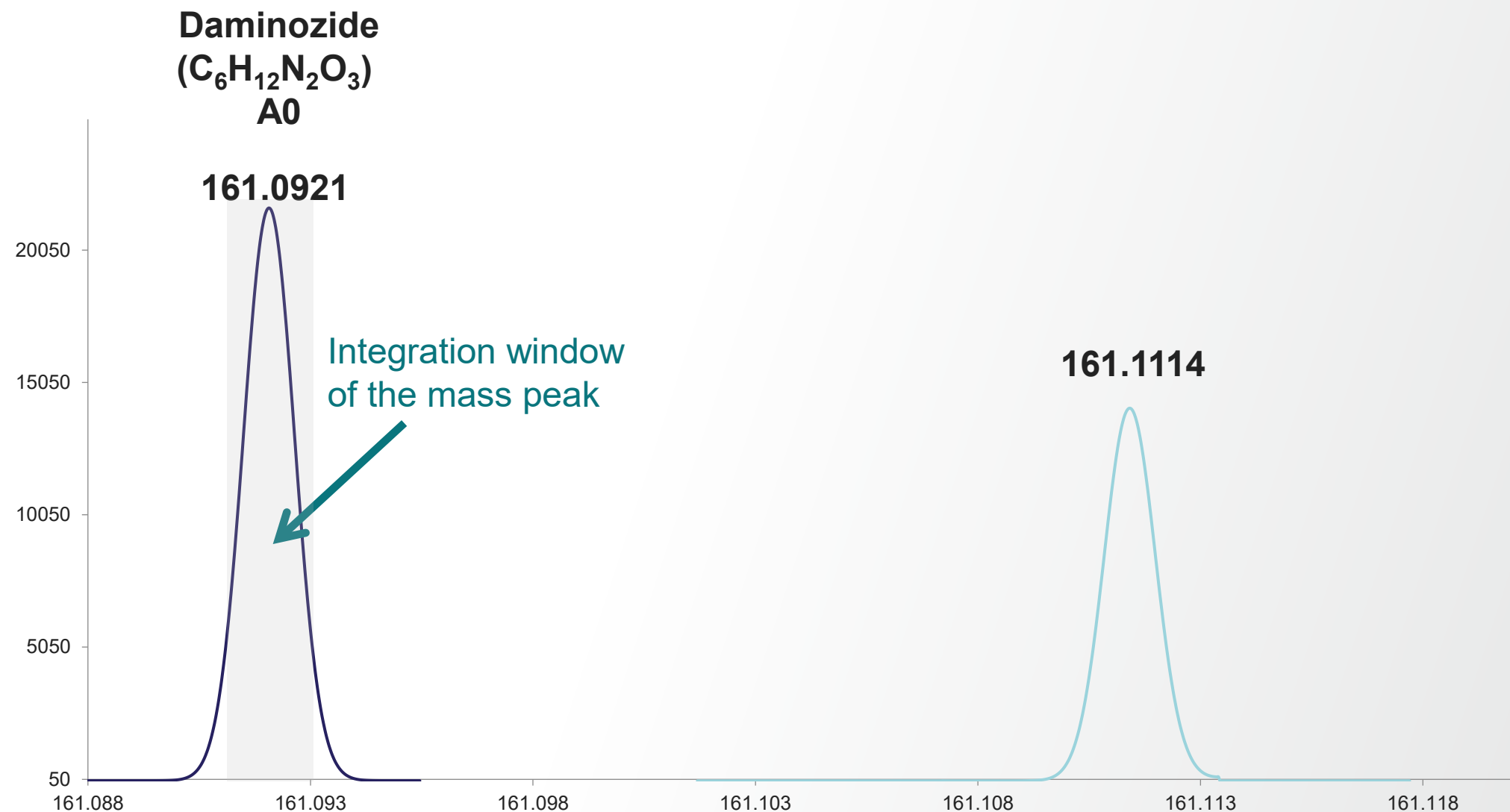
$[M+H]^+$ of Daminozide ($C_6H_{12}N_2O_3$)



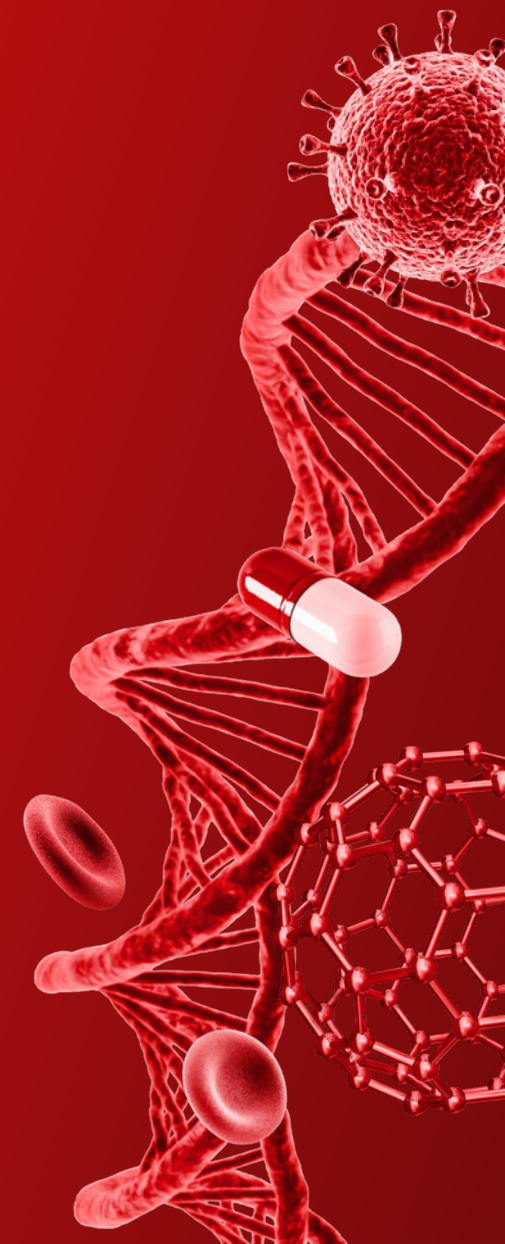
Cross Talk with High Resolution



Cross Talk with High Resolution



Speed

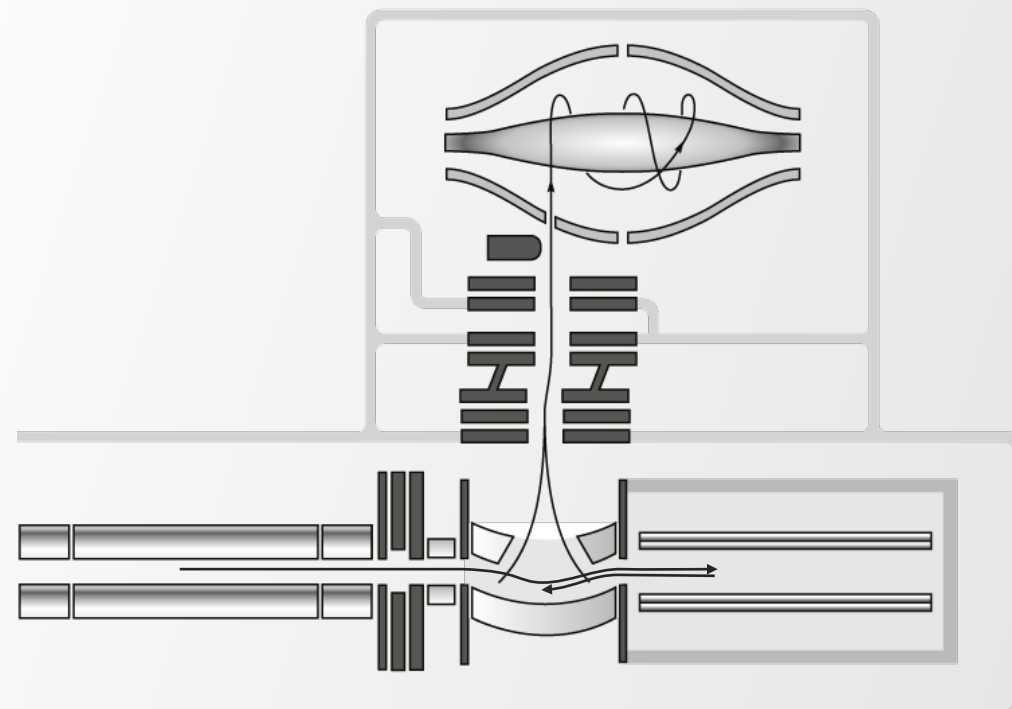


Orbitrap Acquisition Rates

- How fast do you want to go?

- *The selection of the resolution does not affect the sensitivity, just the acquisition rate*

Resolution at m/z 200	Acquisition Rate (Hz)	Acquisition Time (ms)
15,000	22	45
30,000	12	83
45,000	9	111
60,000	6	167
120,000	3	333
240,000	1.5	667



Orbitrap Acquisition Rates

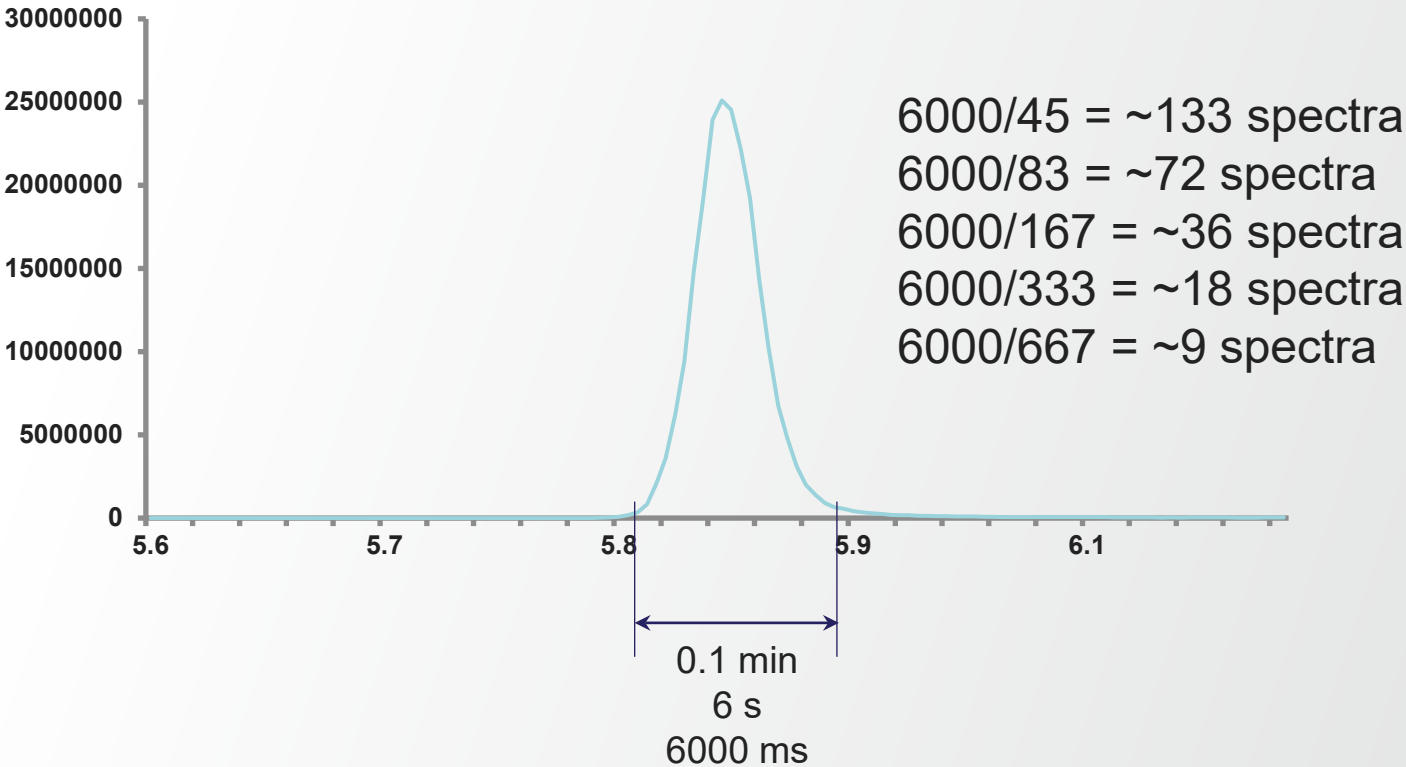


- How fast do you **NEED** to go?

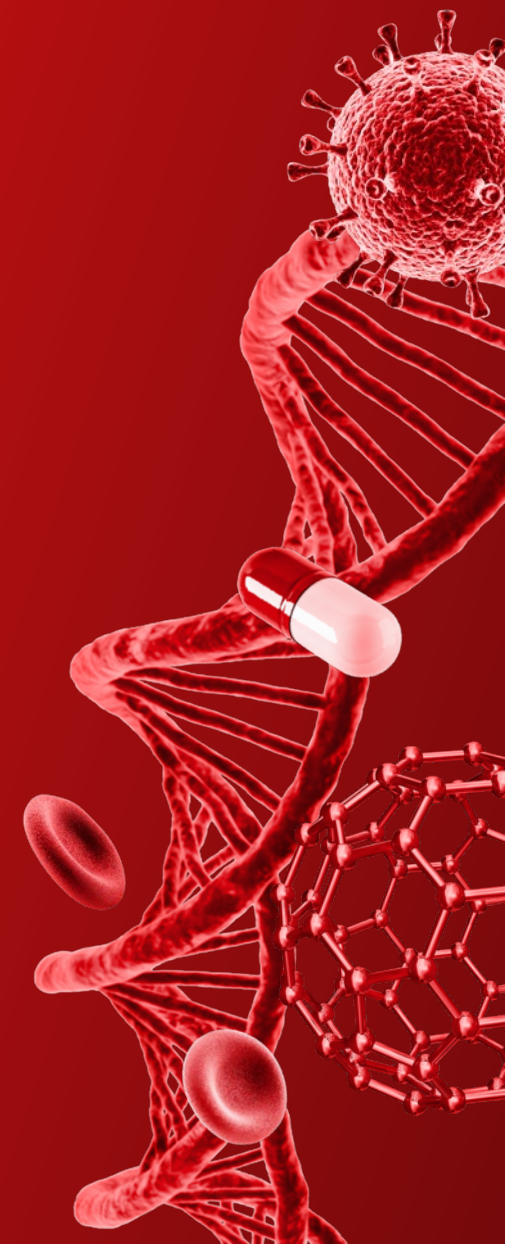
- Ask the chromatogram!

- Quantitation: 10-15 data points (spectra) per chromatographic peak
- Screening: ~4-8 data points (spectra) per chromatographic peak

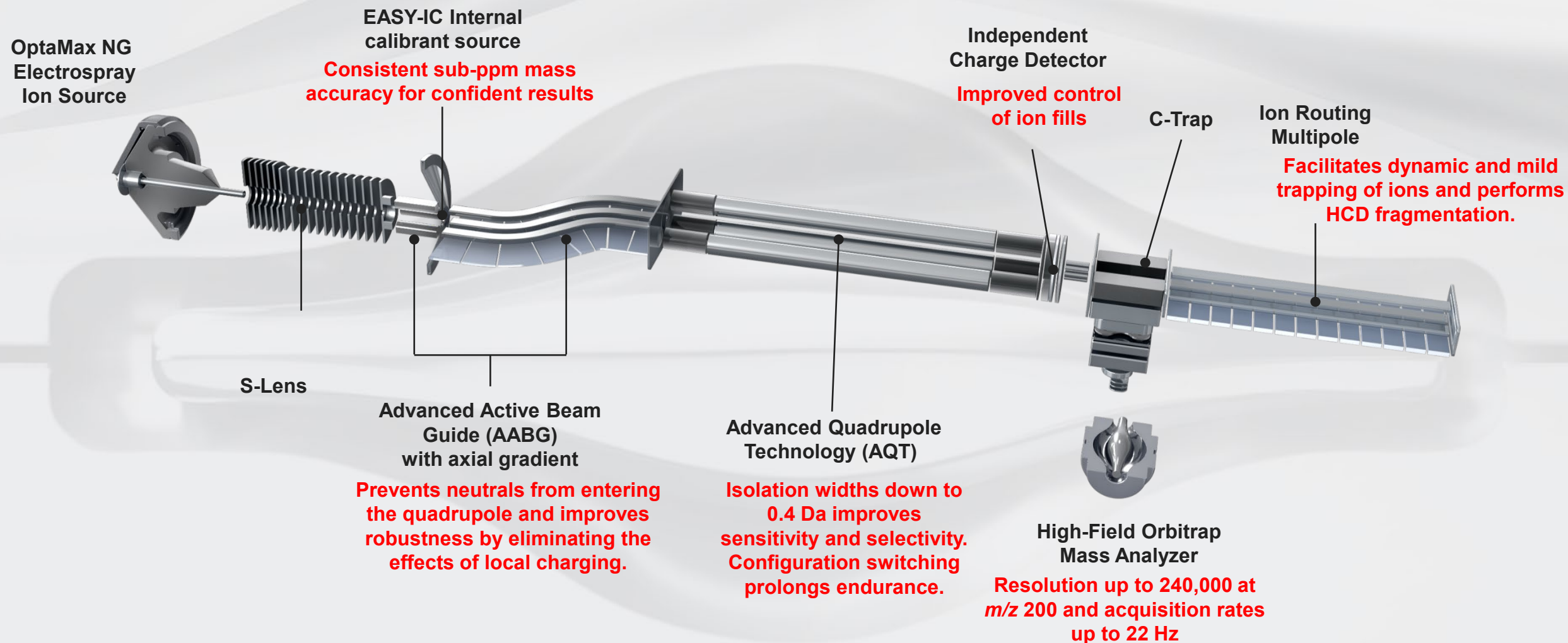
Resolution at m/z 200	Acquisition Rate (Hz)	Acquisition Time(ms)
15,000	22	45
30,000	12	83
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120,000	3	333
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Versatility



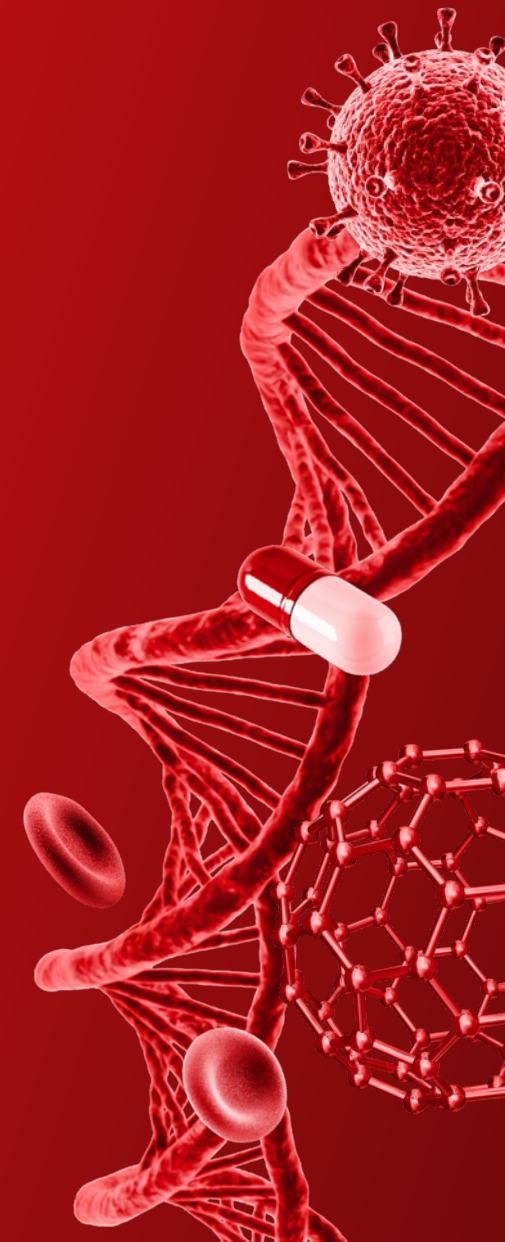
Thermo Scientific Orbitrap Exploris 240 MS Schematic



Orbitrap Exploris Experiments

- FullMS – High Resolution Accurate Mass (HRAM) spectra across a defined mass range
- SIM – Select Ion Monitoring
- Product Ion – MS/MS (MS2) – fragmentation of a selected precursor ion and collecting all the fragments
- FullMS ddMS2 – targeted and non-targeted experiments where product ion experiments are directed by ions observed in the FullMS spectrum
- AIF – all ion fragmentation – product ion experiments on a selected m/z bandwidth of ions
- DIA – data independent product ion experiments on multiple sequentially selected m/z bandwidths of ions

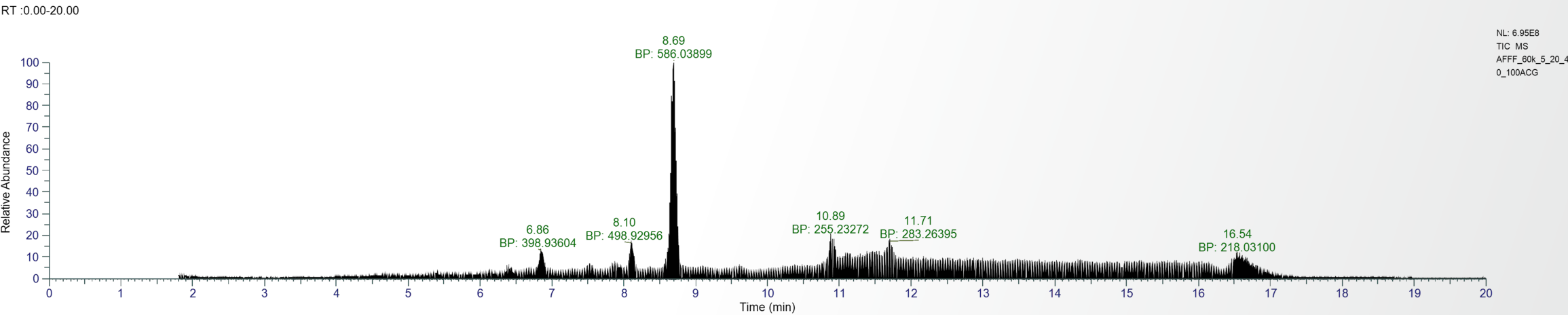
Mass Accuracy AND Precision



FuIMS-ddMS2 of PFAS mix



(collect a mass spectrum, trigger MS2 based on the observed ions, repeat)

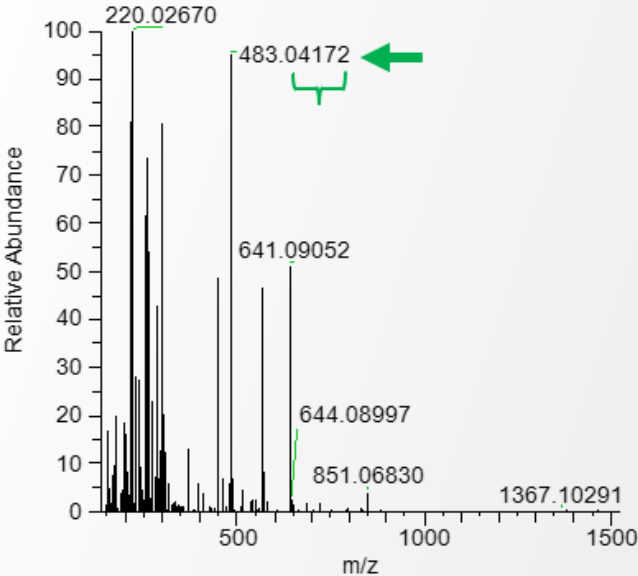
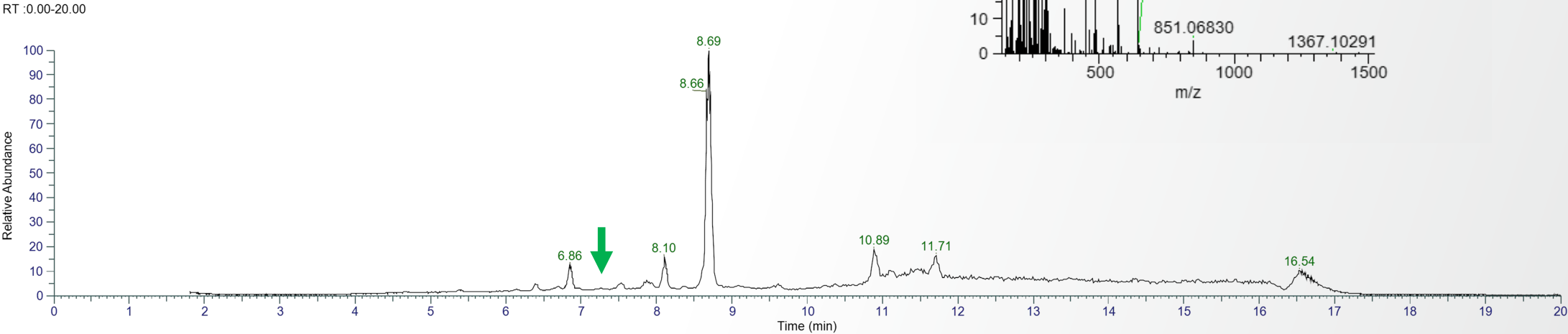


Data from Sarah Choyke and Chris Higgins at the CO School of Mines

Data filtered for only MS experiments



ACG #4534 RT: 7.31 AV: 1 NL: 7.73E5
T: FTMS - c ESI Full ms [150.0000-1500.0000]



NL: 6.95E8
TIC MS F: FTMS - c
ESI Full ms
[150.0000-1500.0000]
ACG

Extracted Ion Chromatogram for m/z 483.04172

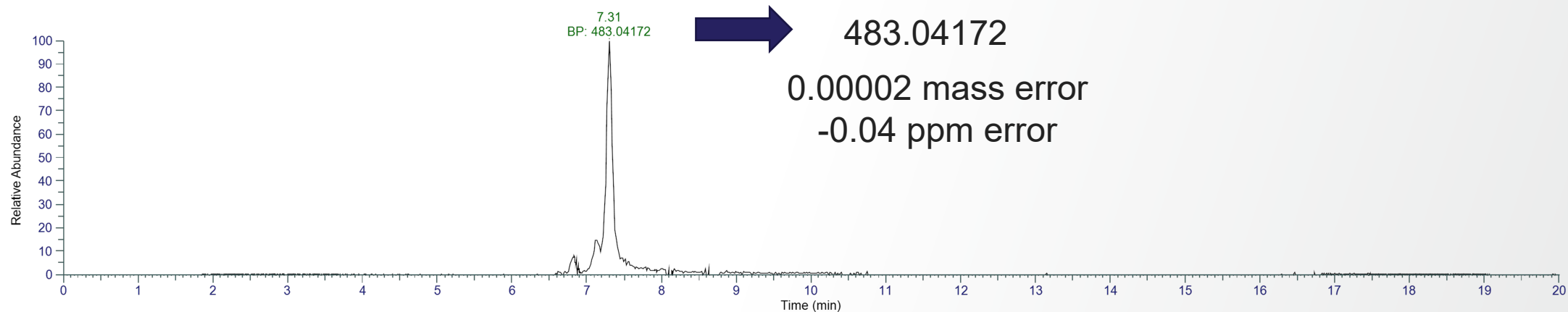
6:2 fluorotelomer sulfonamido propyl amine

$C_{11}H_{13}F_{13}N_2O_2S$

MW = 484.04901

$[M-H]^- = 243.04174$

RT : 0.00-20.00

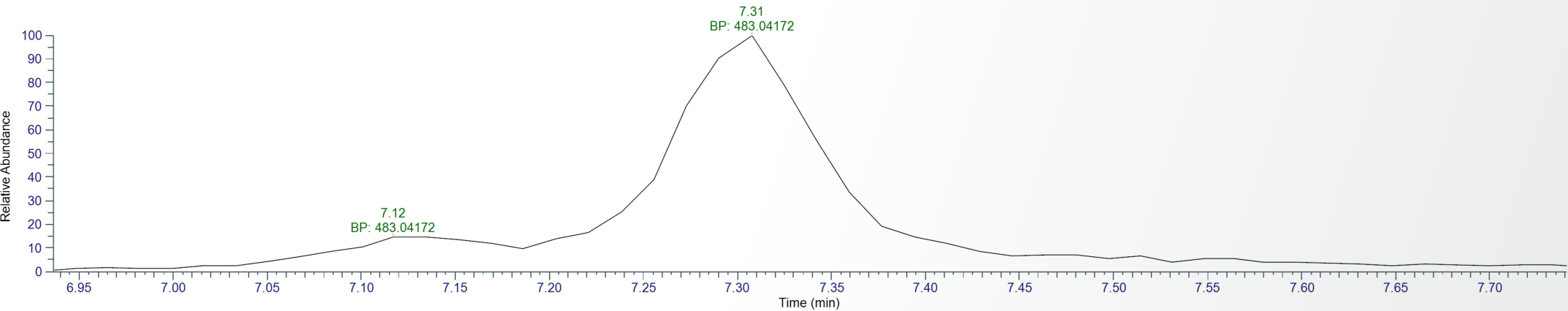


NL: 7.36E5
m/z= 483.03928-483.04412 MS
F: FTMS - c ESI Full ms
[150.0000-1500.0000]
AFFF_60k_5_20_40_100ACG

“Mass Accuracy”

Extracted Ion Chromatogram for *m/z* 483.04172

RT: 6.94-7.74



NL: 7.36E5
m/z= 483.03928-483.04412 MS
F: FTMS - c ESI Full ms
[150.0000-1500.0000]
AFFF_60k_5_20_40_100ACG

“Stick” Mode Plotting of Chromatogram

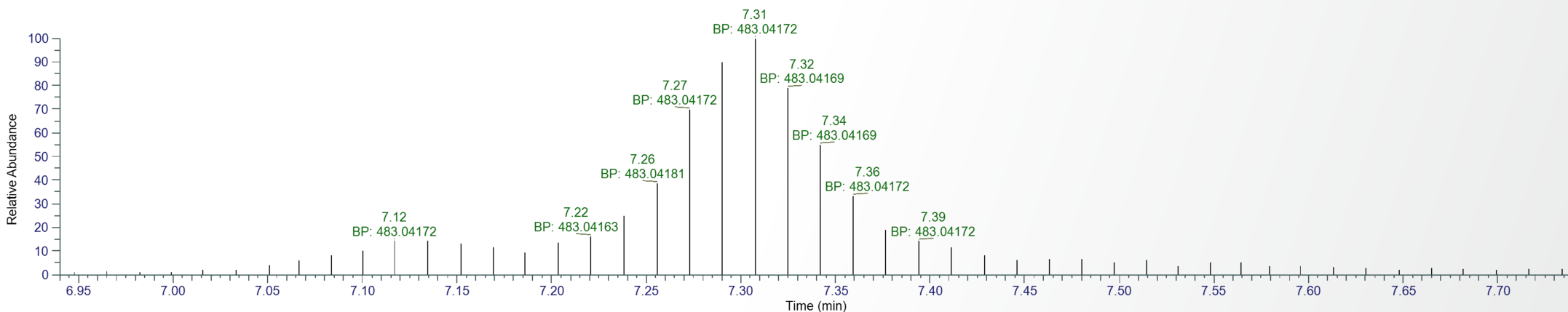
6:2 fluorotelomer sulfonamido propyl amine

$C_{11}H_{13}F_{13}N_2O_2S$

MW = 484.04901

$[M-H]^- = 243.04174$

RT: 6.94-7.74



NL: 7.36E5
m/z= 483.03928-483.04412 MS
F: FTMS - c ESI Full ms
[150.0000-1500.0000]
AFFF_60k_5_20_40_100ACG

“Stick” Mode Plotting of Chromatogram

6:2 fluorotelomer sulfonamido propyl amine

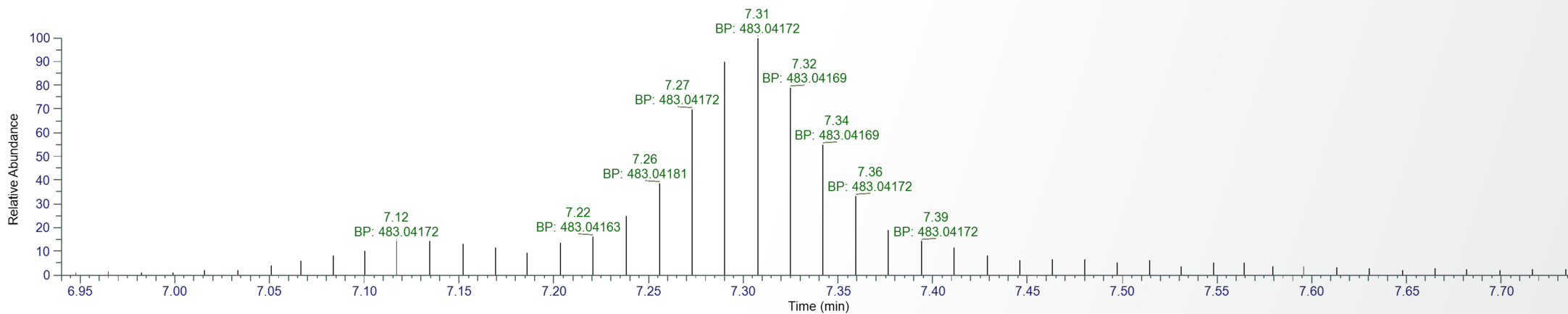
$C_{11}H_{13}F_{13}N_2O_2S$

MW = 484.04901

$[M-H]^- = 243.04174$

RT: 6.94-7.74

NL: 7.36E5
m/z= 483.03928-483.04412 MS
F: FTMS - c ESI Full ms
[150.0000-1500.0000]
AFFF_60k_5_20_40_100ACG



“Stick” Mode Plotting of Chromatogram

6:2 fluorotelomer sulfonamido propyl amine



MW = 484.04901

$[\text{M}-\text{H}]^- = 243.04174$

Spread is 0.373 ppm



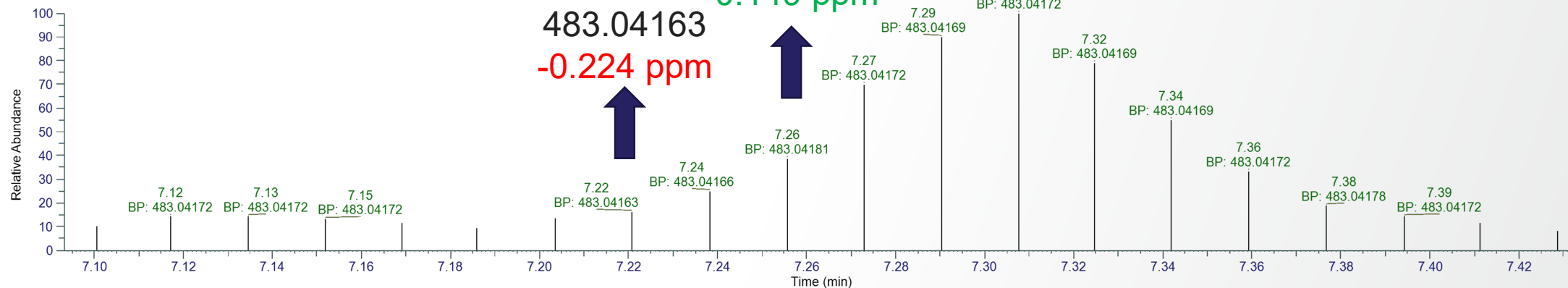
483.04181

0.149 ppm

483.04163
-0.224 ppm



RT : 7.09-7.43



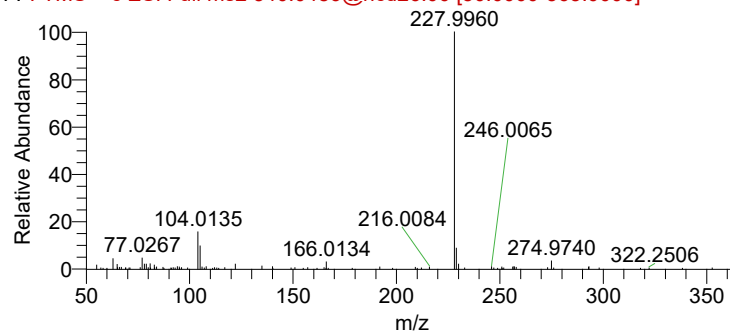
NL: 7.36E5
m/z= 483.03928-483.04412 MS
F: FTMS - c ESI Full ms
[150.0000-1500.0000]
AFFF_60k_5_20_40_100ACG

“Mass Accuracy AND Precision”

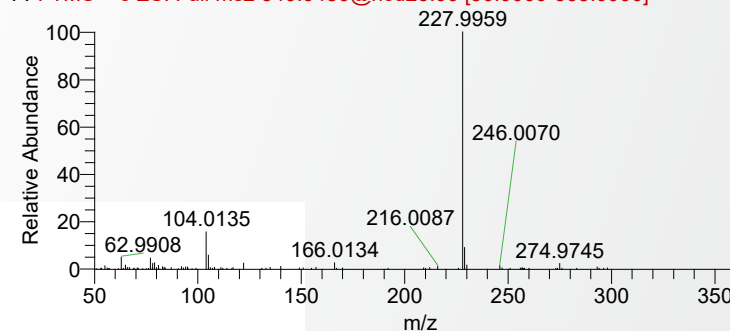
HRAM PRM LC/MS of Mesotrione

– Consistent MS/MS Across Chromatographic Peak

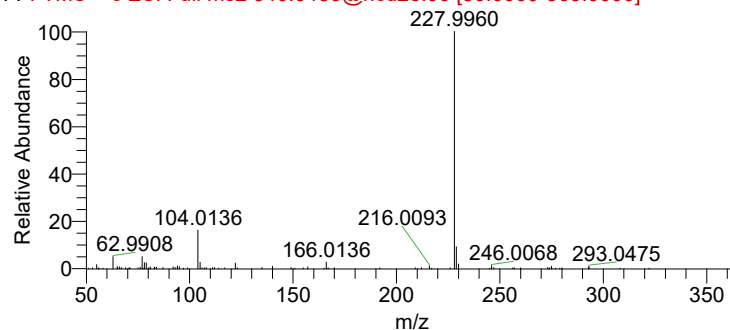
Dicam-Meso_PRM_036 #377 RT: 3.3034 AV: 1 NL: 9.60E4
F: FTMS + c ESI Full ms2 340.0486@hcd26.00 [50.0000-365.0000]



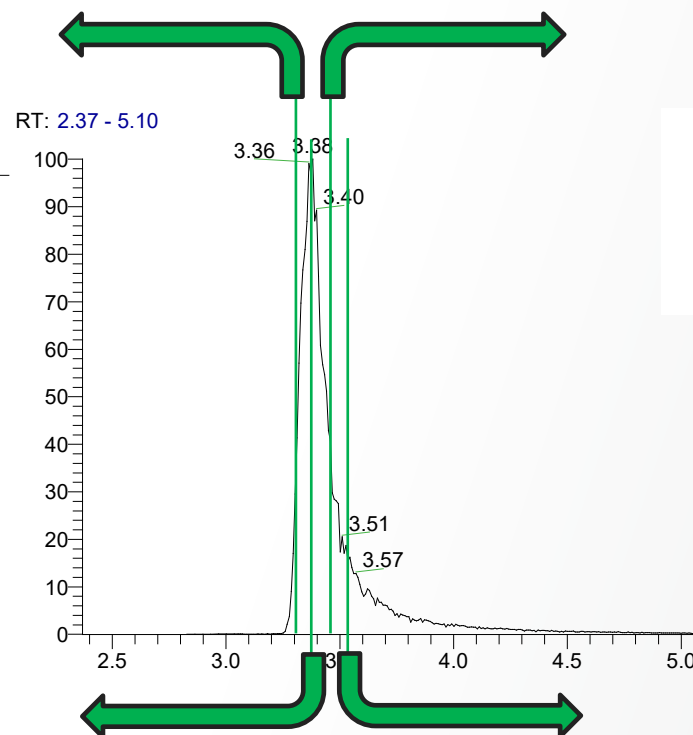
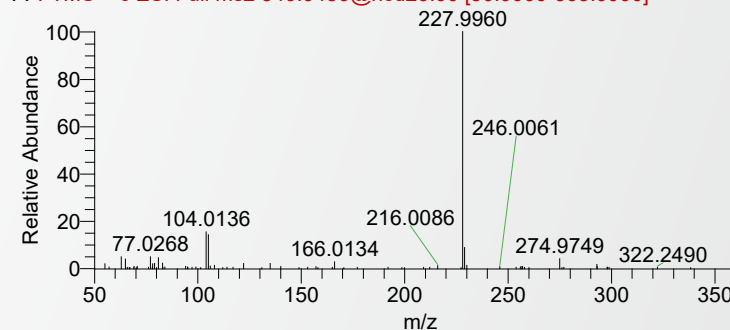
Dicam-Meso_PRM_036 #393 RT: 3.4412 AV: 1 NL: 1.66E5
F: FTMS + c ESI Full ms2 340.0486@hcd26.00 [50.0000-365.0000]



Dicam-Meso_PRM_036 #385 RT: 3.3723 AV: 1 NL: 3.15E5
F: FTMS + c ESI Full ms2 340.0486@hcd26.00 [50.0000-365.0000]



Dicam-Meso_PRM_036 #401 RT: 3.5100 AV: 1 NL: 6.67E4
F: FTMS + c ESI Full ms2 340.0486@hcd26.00 [50.0000-365.0000]



Summary

- Orbitraps are very cool and powerful devices
- Orbitraps have plenty of acquisition speed for high resolution LC/MS applications
- Orbitraps have multiple useful acquisition modes
- The mass accuracy and precision (without the need for averaging) of the Orbitrap Exploris family of instruments is phenomenal, amazingly consistent from spectrum to spectrum, and is proven in the field in the hands of our customers.
- MS2 spectra are reproducible (without the need for averaging) across the entire chromatographic peak

Thank you!

