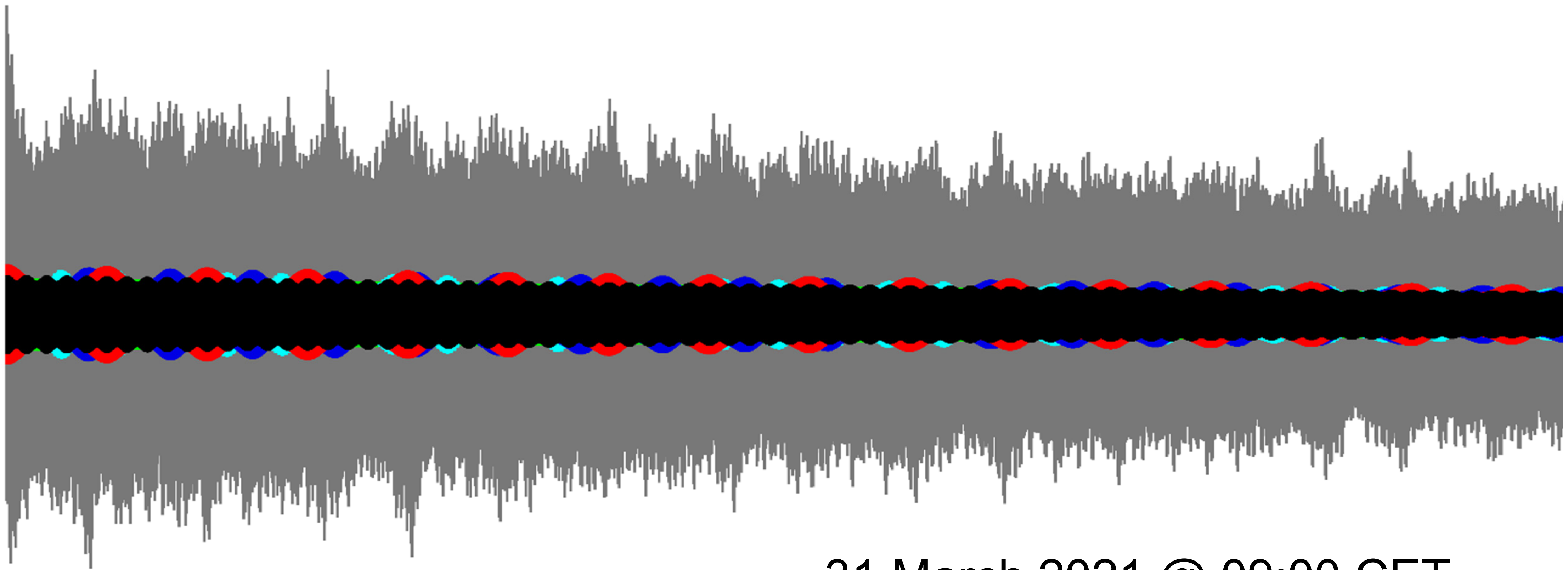
Spectroswiss
FTMS Science and Technology

XXVème Rencontres du Club Jeune SFSM 2021

Fourier Transform Mass Spectrometry: Fundamentals and Data Processing



Yury Tsybin
tsybin@spectroswiss.ch

Spectroswiss
Lausanne, Switzerland

31 March 2021 @ 09:00 CET

FTMS: Fundamentals and Data Processing

I. FTMS Fundamentals: General

II. FT-ICR MS / MRMS: Principles of Operation

III. Orbitrap FTMS: Principles of Operation

IV. FTMS Data Processing

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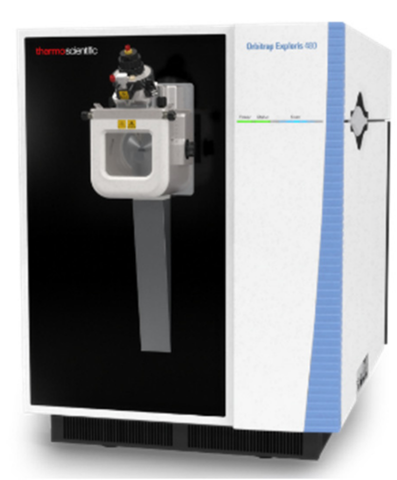
Fourier Transform Mass Spectrometry: **FTMS**

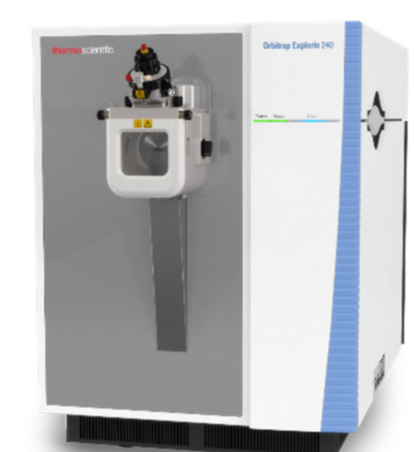
ICR: ion cyclotron resonance

MRMS: magnetic resonance MS

Orbitraps

Electrostatic ion traps





FTMS Principles

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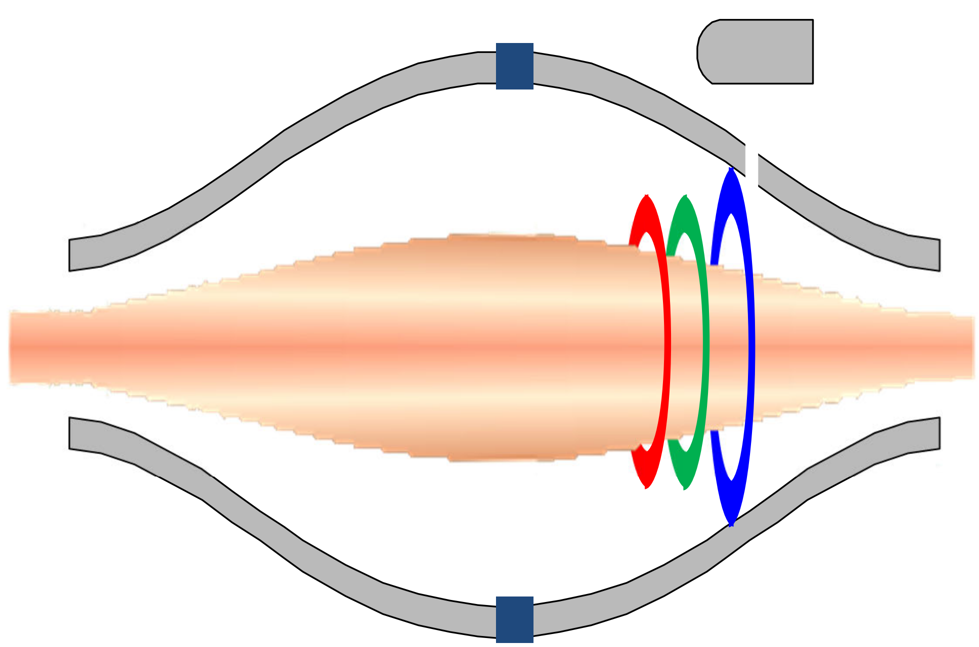
- Ion identity (*m/z*) is encoded as a frequency of ion oscillations in an ion trap
- Frequencies of ion oscillations are measured as time-domain signals (**transients**)
- Fourier transform (FT) decodes transients to reveal frequencies (*m/z*) values

Electrostatic field-based

Orbitrap



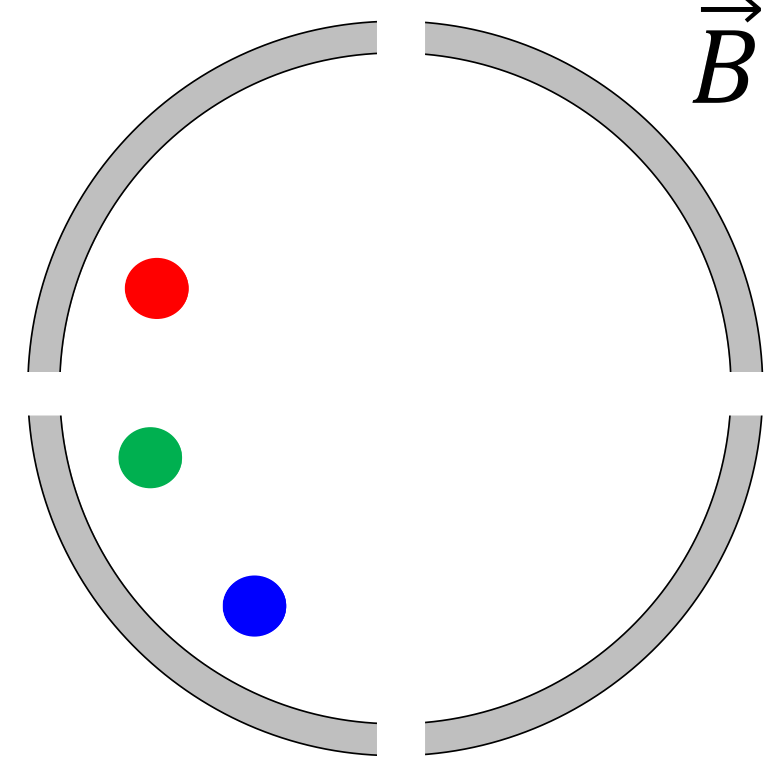
$$\omega \approx \sqrt{\frac{k}{m/z}}$$

Orbitrap™ families: LTQ Orbitrap; Exactive; Q Exactive; Exploris; Fusion; Lumos; Eclipse

Magnetic field-based

Ion Cyclotron Resonance (ICR)

Magnetic Resonance MS (MRMS)



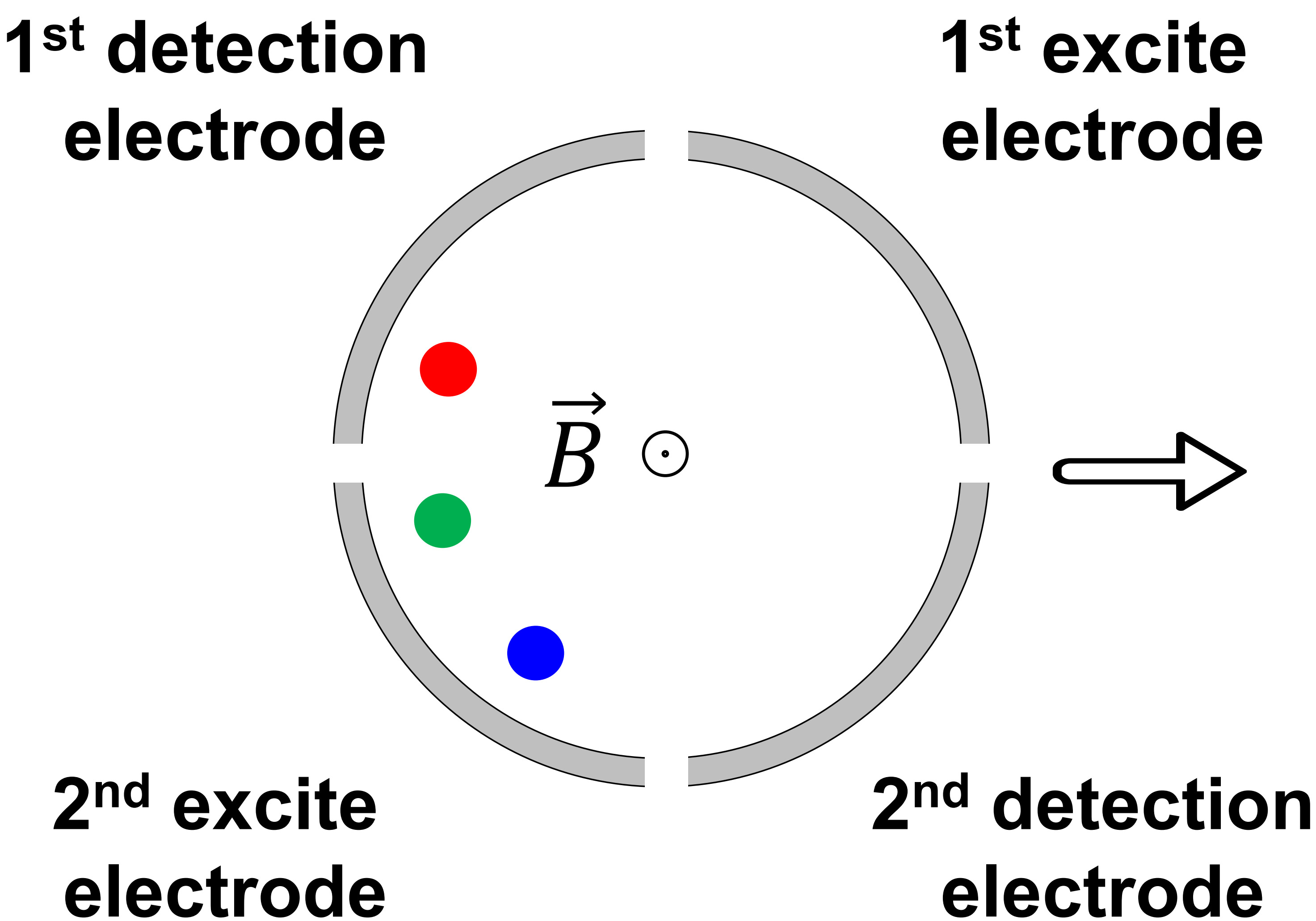
$$\vec{B} \odot$$

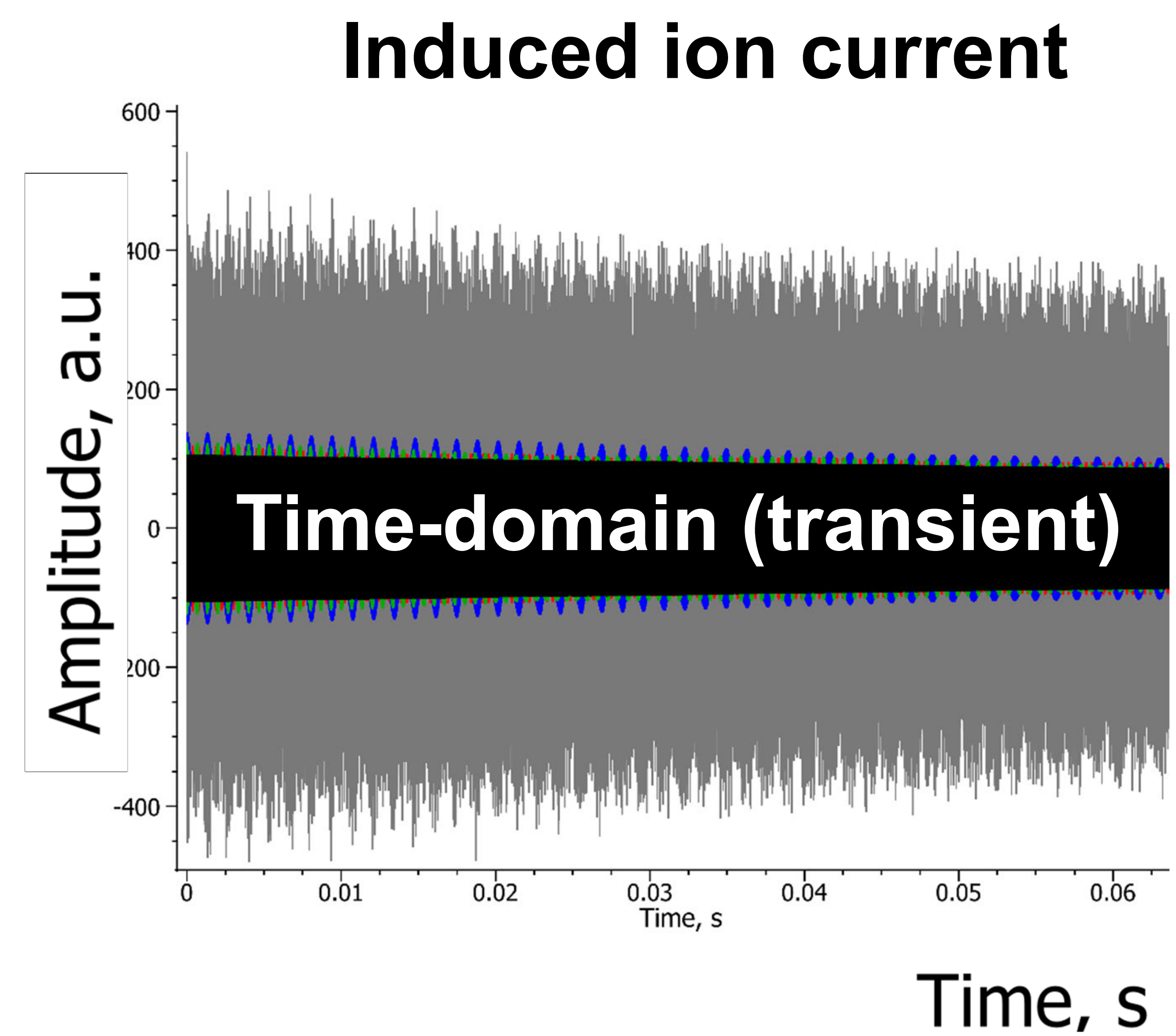
$$\omega \approx \frac{1}{m/z}$$

LTQ FT
Apex
SolariX
ScimaX

From Ion Oscillations to Ion Signals: **FT-ICR MS**

$$\omega \approx \frac{1}{m/z}$$





FT

From Ion Oscillations to Ion Signals: **Orbitrap FTMS**

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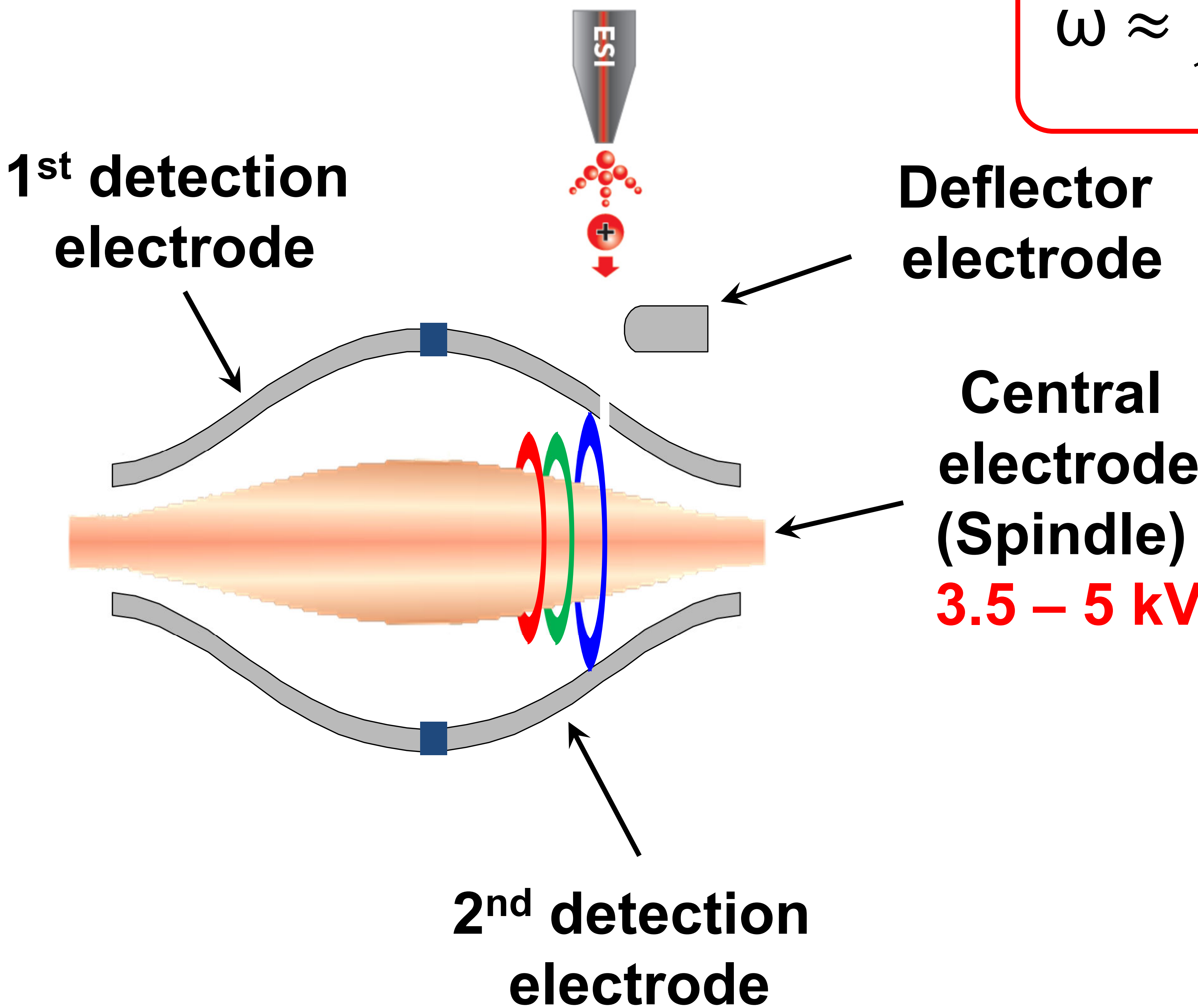
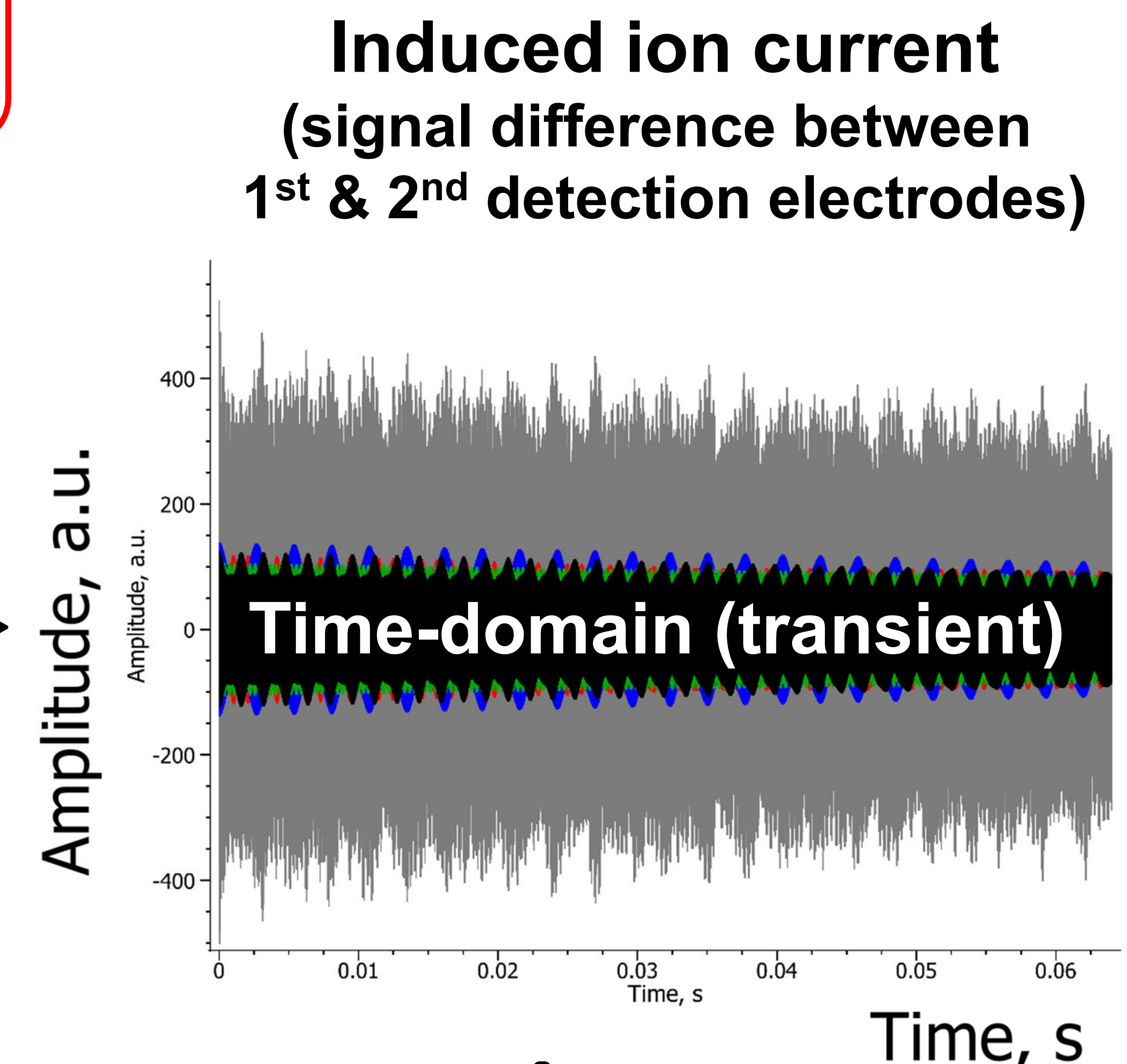
$$\omega \approx \sqrt{\frac{k}{m/z}}$$





FT

Fourier Transform (**FT**): From Transients to Frequencies

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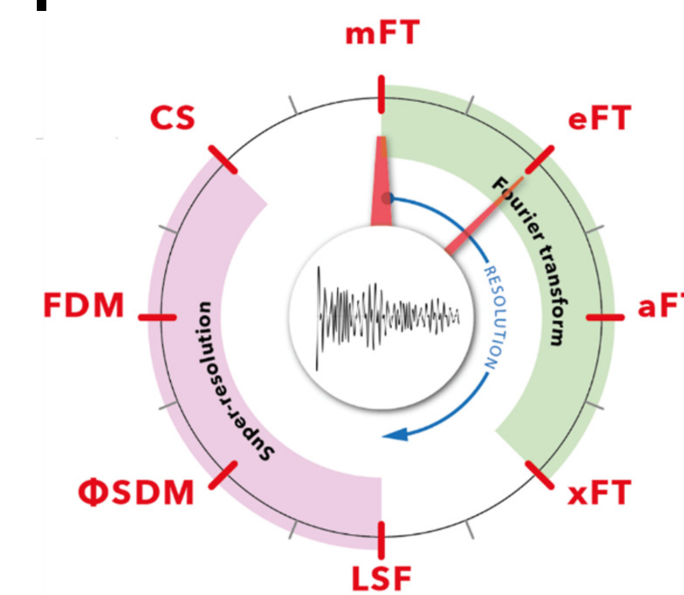

- General information on FT processing:
  - https://www.youtube.com/watch?v=spUNpyF58BY
- Magnitude FT (**mFT**): basic and most common approach
  - all FT-ICR MS / MRMS and earlier Orbitraps (up to and including LTQ Orbitrap Velos)
  - Data processing in FTMS: O'Connor *et al*., *Mass Spectrom. Reviews* (2014) 33:333
- Enhanced FT (**eFT**): a combination of mFT (peak bottom) and aFT (peak top)
  - all Orbitraps starting with LTQ Orbitrap Elite (Makarov *et al*., *IJMS* (2014) 369, 16-22)
- Absorption FT (**aFT**): doubles mFT resolution, information equal to transients
  - post-processing of transients (*e.g*., with AutoVectis, see www.kilgourlab.com)
  - in-hardware via acquisition of phased transients (*e.g*., DOI: 10.1021/jasms.9b00032)

Frequency - *m/z* Relationships: Calibration

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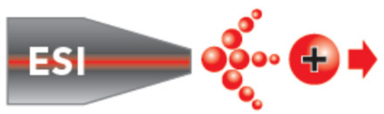

Ions, m/z

Orbitrap

$$\omega \approx \sqrt{\frac{k}{m/z}}$$

FT-ICR MS / MRMS

$$\omega \approx \frac{1}{m/z}$$

Ions	m/z	*f, kHz* @ QE HF	*f, kHz* @ 12 T
S	106	1413	1738
SF	253	915	728
SFS	340	789	542
SFSM	471	670	391

- What is *k*?

Ion oscillation frequency reduces FASTER for ICR compared to Orbitrap

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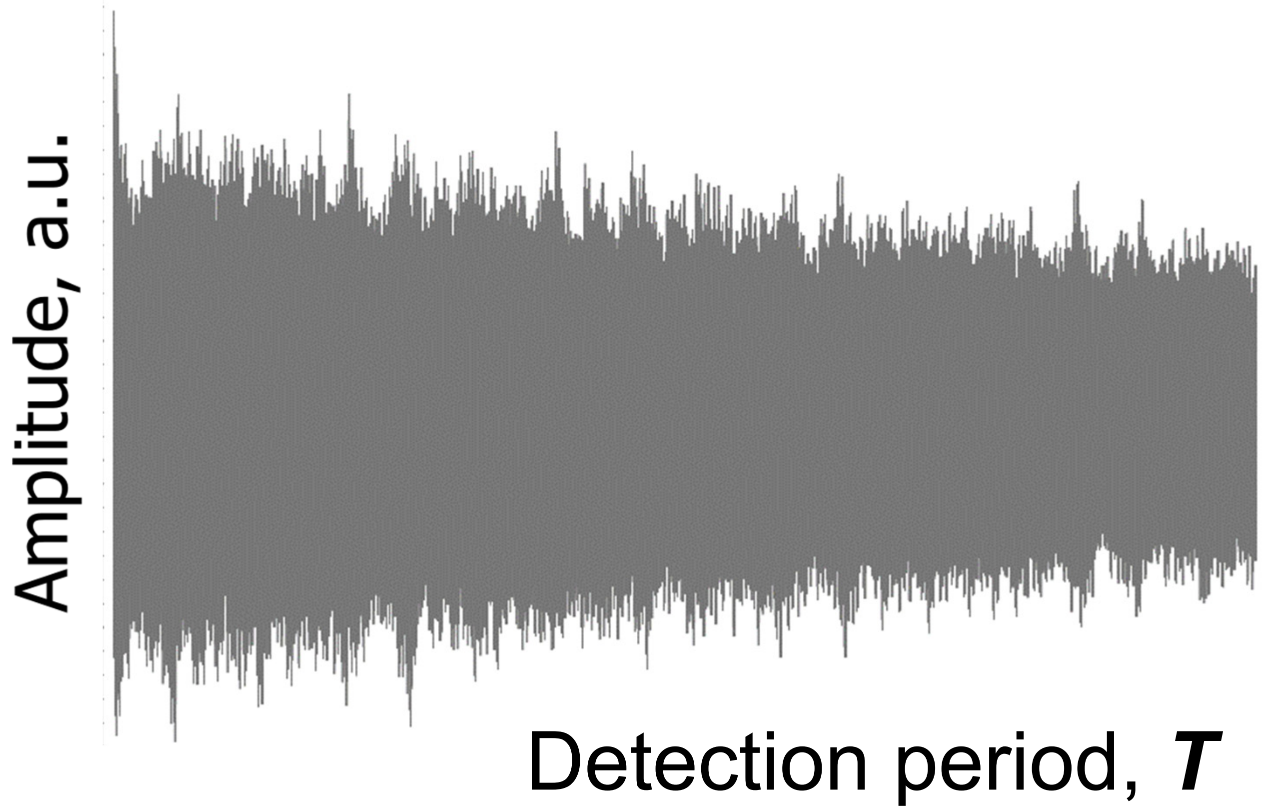
FTMS Data Processing Example

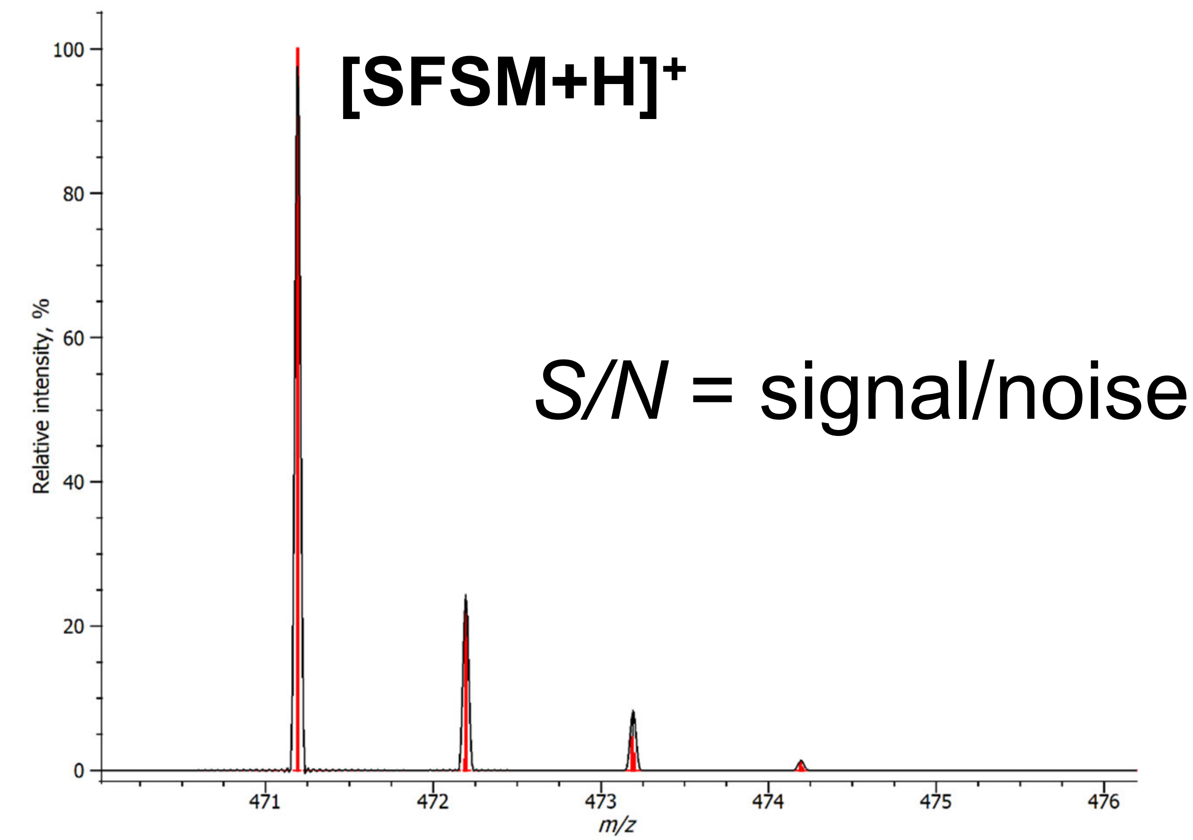
Time-domain ion signals (transients)



FT

calibration

Absorption mode mass spectra



$R \sim T$ • Resolution increases linearly with transient length (detection period)

$S/N \sim \sqrt{T}$ • Sensitivity increases as a sqrt of transient length (detection period)

$S/N \sim z$ • Peak intensities are directly proportional to the charge state of the ions

$S/N(t) \sim z$ • Peak intensity increase in time is proportional to the ion's charge state

Individual ion counting (charge detection FTMS): DOI: 10.1038/s41592-020-0764-5

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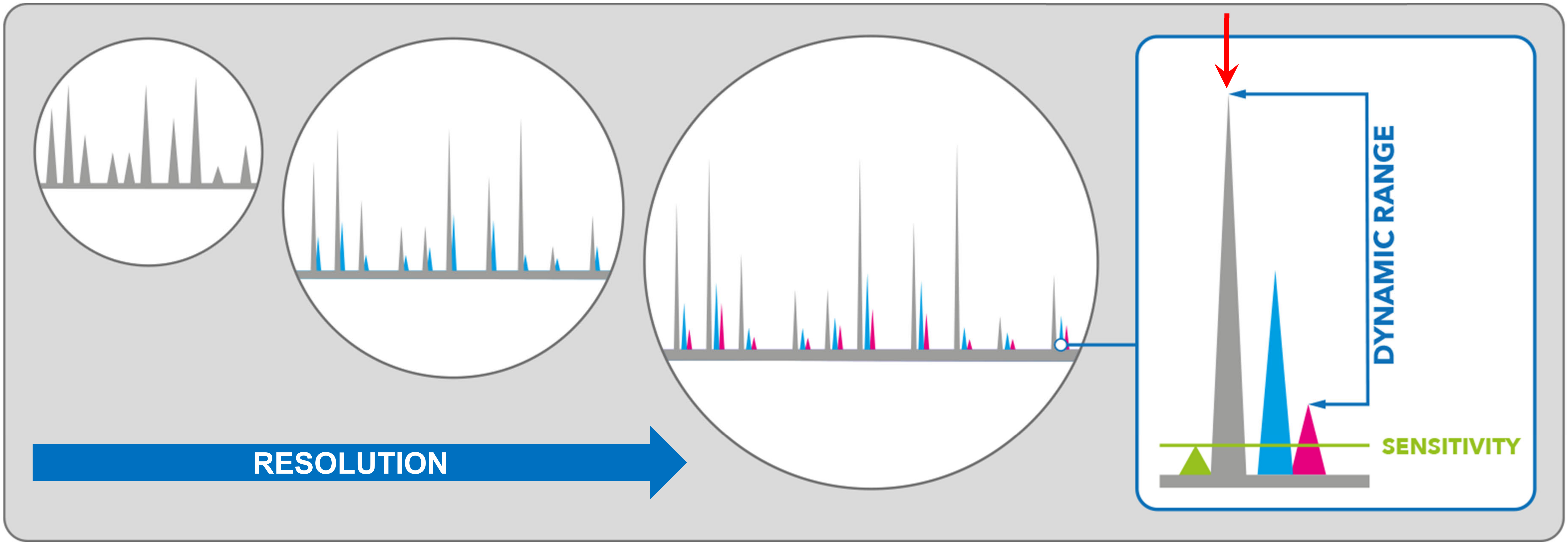
FTMS Analytical Characteristics

- **the highest resolution**
- **the highest mass accuracy**

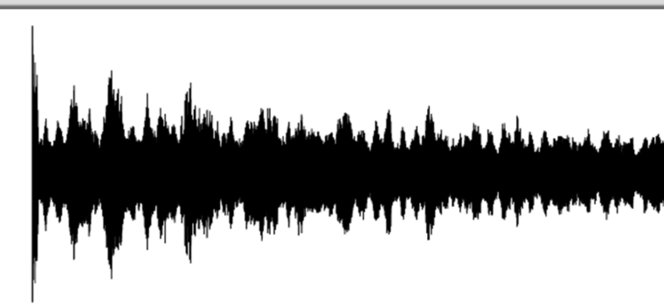
ABUNDANCE ACCURACY

MASS ACCURACY



DATA ACQUISITION SPEED (THROUGHPUT)

induced current ion detection (transients)



$$R \propto f \cdot T$$

(Some) Key Applications of FTMS

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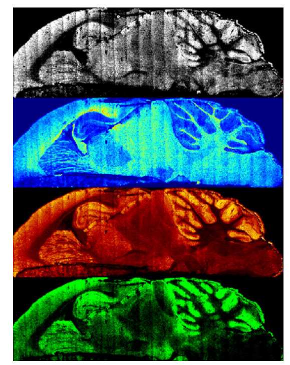
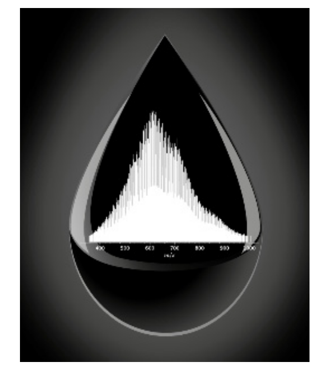
ICR / MRMS

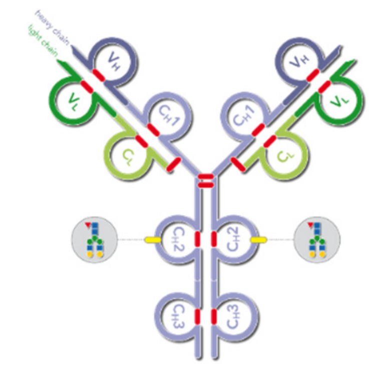
- Ultra-high performance
- High space-charge tolerance
- Ion detection & transformation



Imaging

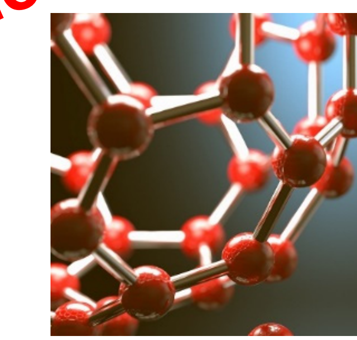


Complex mixture analysis



Structural biology: top-down analysis

In-cell reactions!



Basic science

C.04: Frédéric Aubriet

Orbitraps

- High performance
- Ion detection (only)
- Extremely versatile
- On-line LC/GC/…
- Easy to use (!)

C.02: Sophie Ayciriex

O.12: Maroussia Parailloux

Metabolomics

Bottom-up proteomics

Environmental & Food safety

BioPharma (MAM & top-down)

Clinical/ Toxicology

Pharma metabolite ID/profiling

Protein complexes/viruses: single ion counting (CDMS)
Elemental analysis, isotopic ratio analysis
Imaging, (medium) complex mixtures analysis, …

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FT-ICR MS Concept: Ion Cyclotron Frequency

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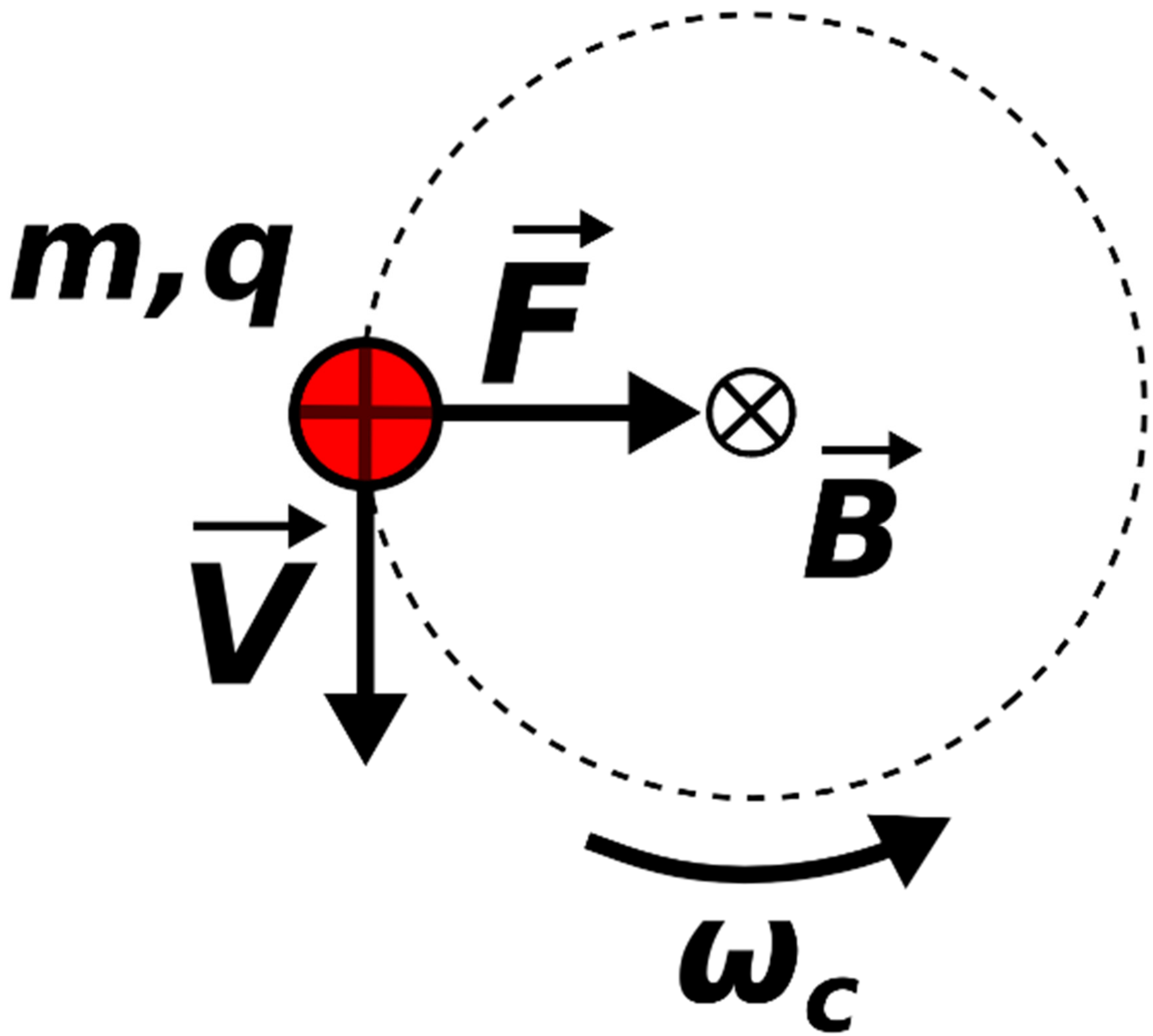
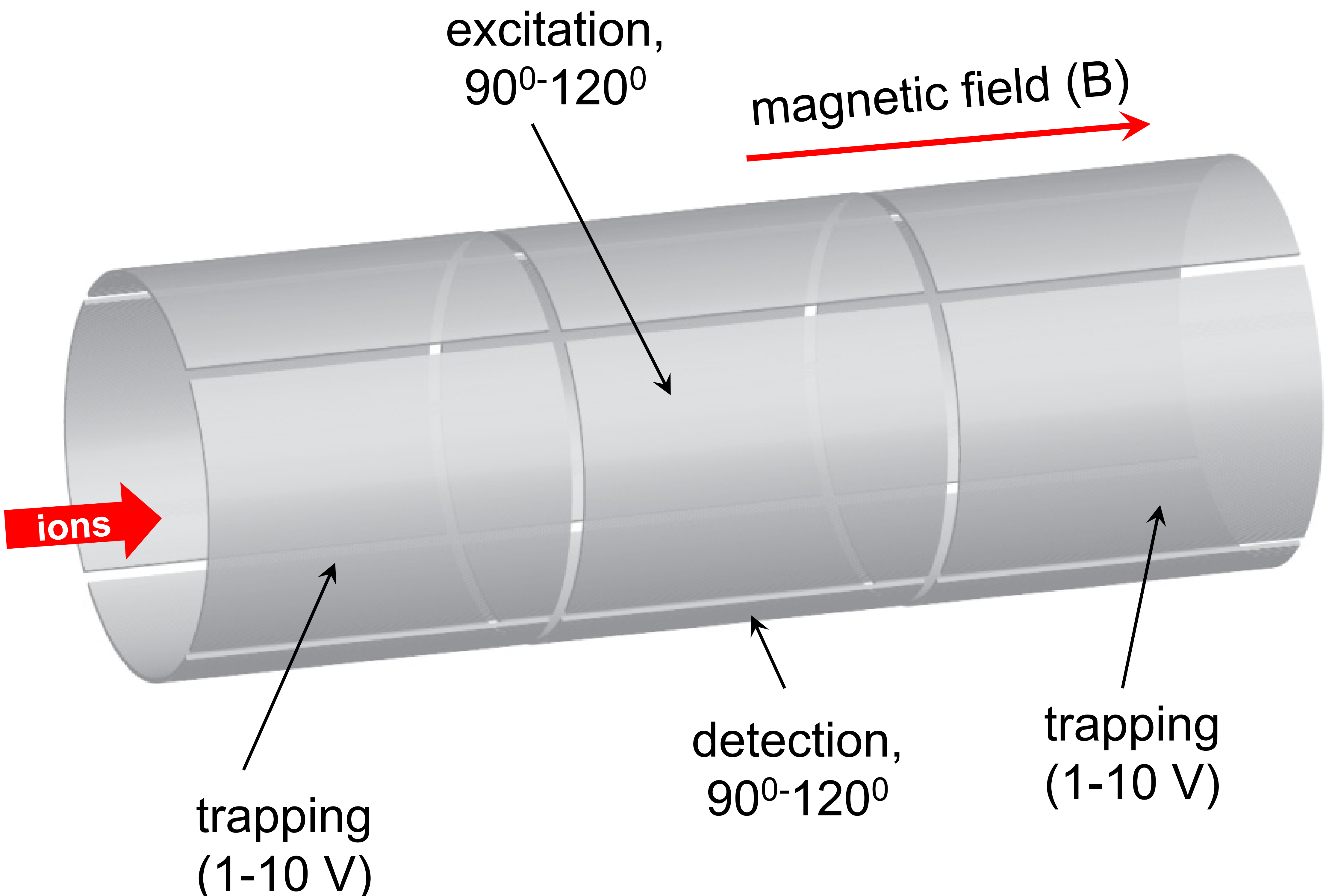


$$\omega_c = \frac{q}{m} B$$

cyclotron frequency

Marshall et al., Mass Spectrometry Reviews (1998) 17:1-35

ICR Ion Trap (Cell): Ion Trapping, Excitation, & Detection

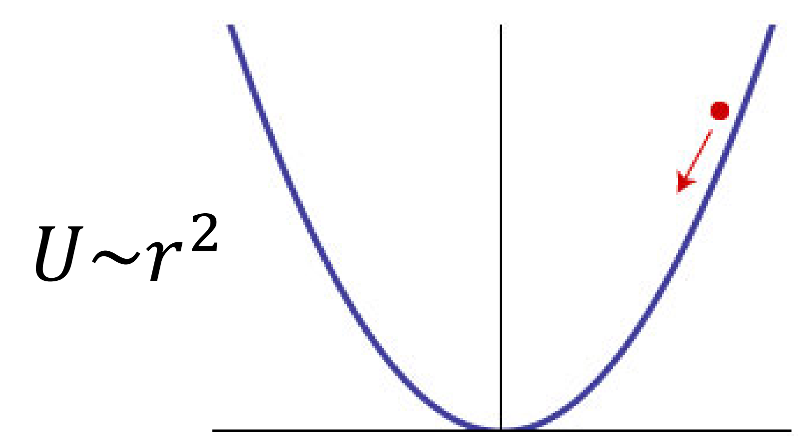


Ion trapping in radial direction:
magnetic field

Ion trapping in axial direction:
electric field

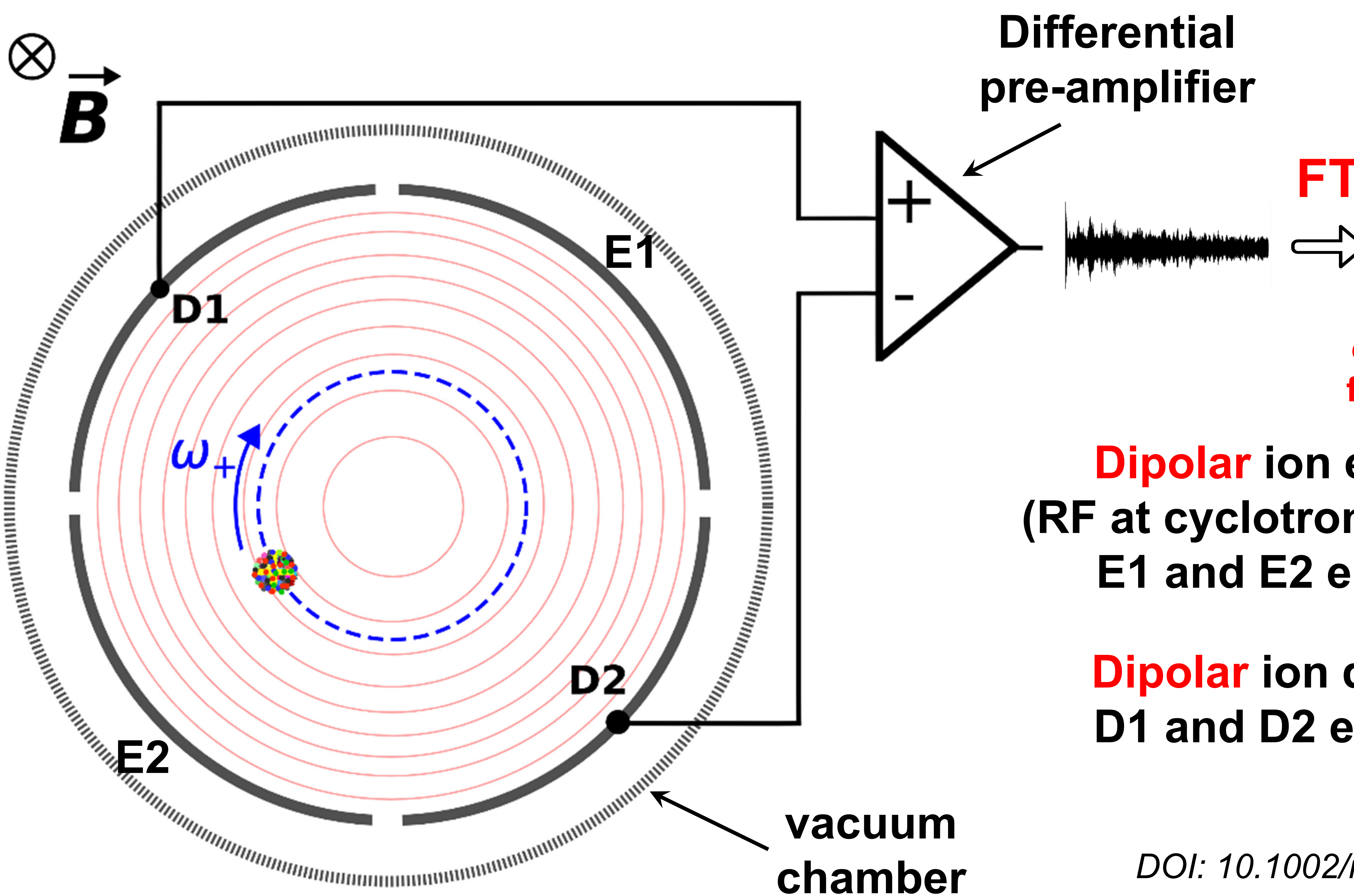
Ideal trapping electric field:
linear field (quadratic trapping potential)

$$E_r = -\frac{d}{dr}U = const \cdot r$$



DOI: 10.1002/mas.21681

Ion Detection in FT-ICR MS



$$\omega_+ = \omega_c - \omega_-$$

reduced cyclotron frequency

magnetron (drift) frequency

Dipolar ion excitation (RF at cyclotron frequency): E1 and E2 electrodes

Dipolar ion detection: D1 and D2 electrodes

DOI: 10.1002/mas.21681

Ion Detection: a Quadratic Trapping Potential

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Ion packet injection

⇩

Ion trapping (on-axis)

⇩

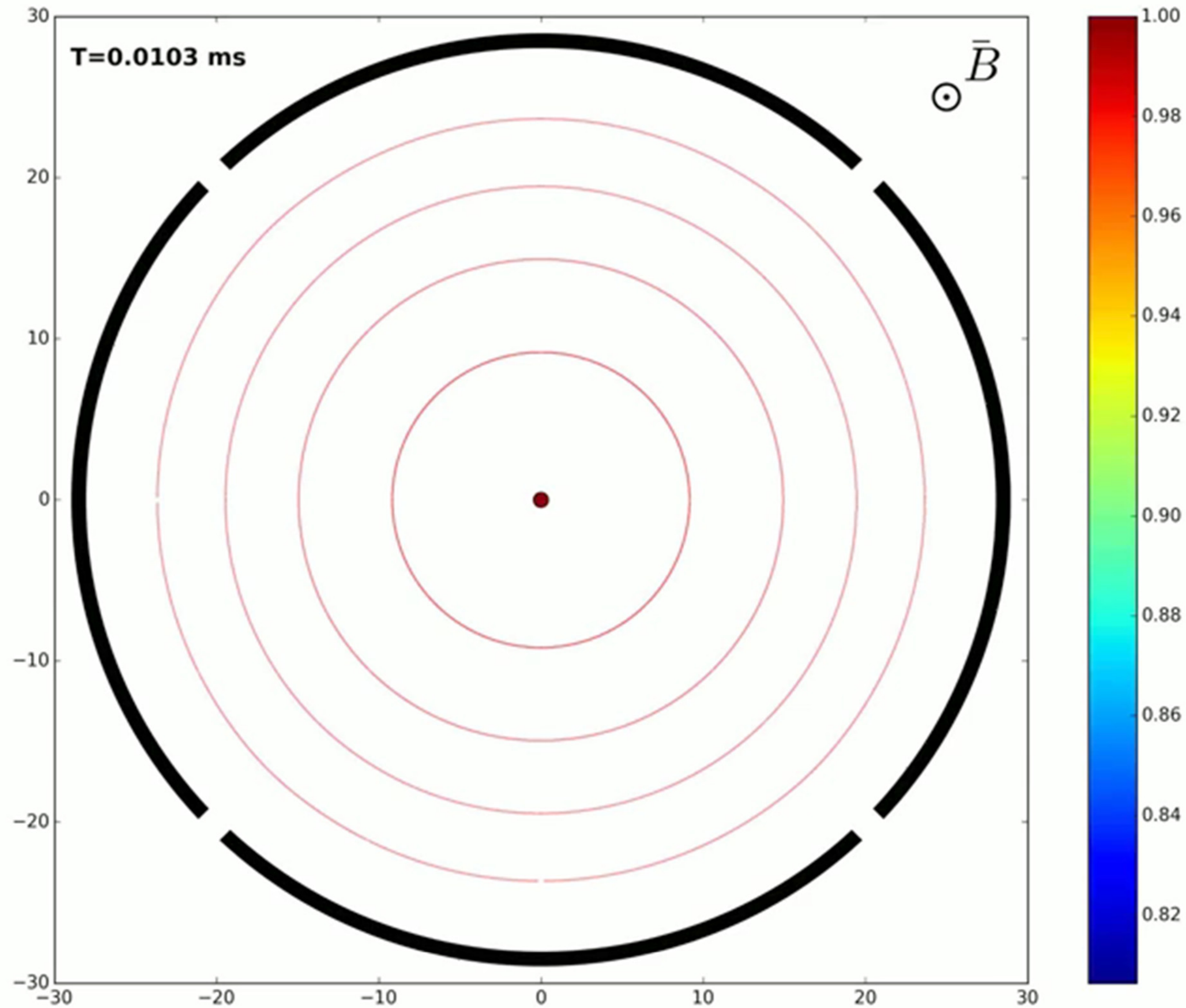
Ion excitation to a higher radius with an RF field (**compact cloud**)

⇩

Ion detection (induced ion current)

⇩

Quench of ions (ion ejection)



Ion Detection: a **Non-Quadratic** Trapping Potential

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Ion packet injection

⇩

Ion trapping (on-axis)

⇩

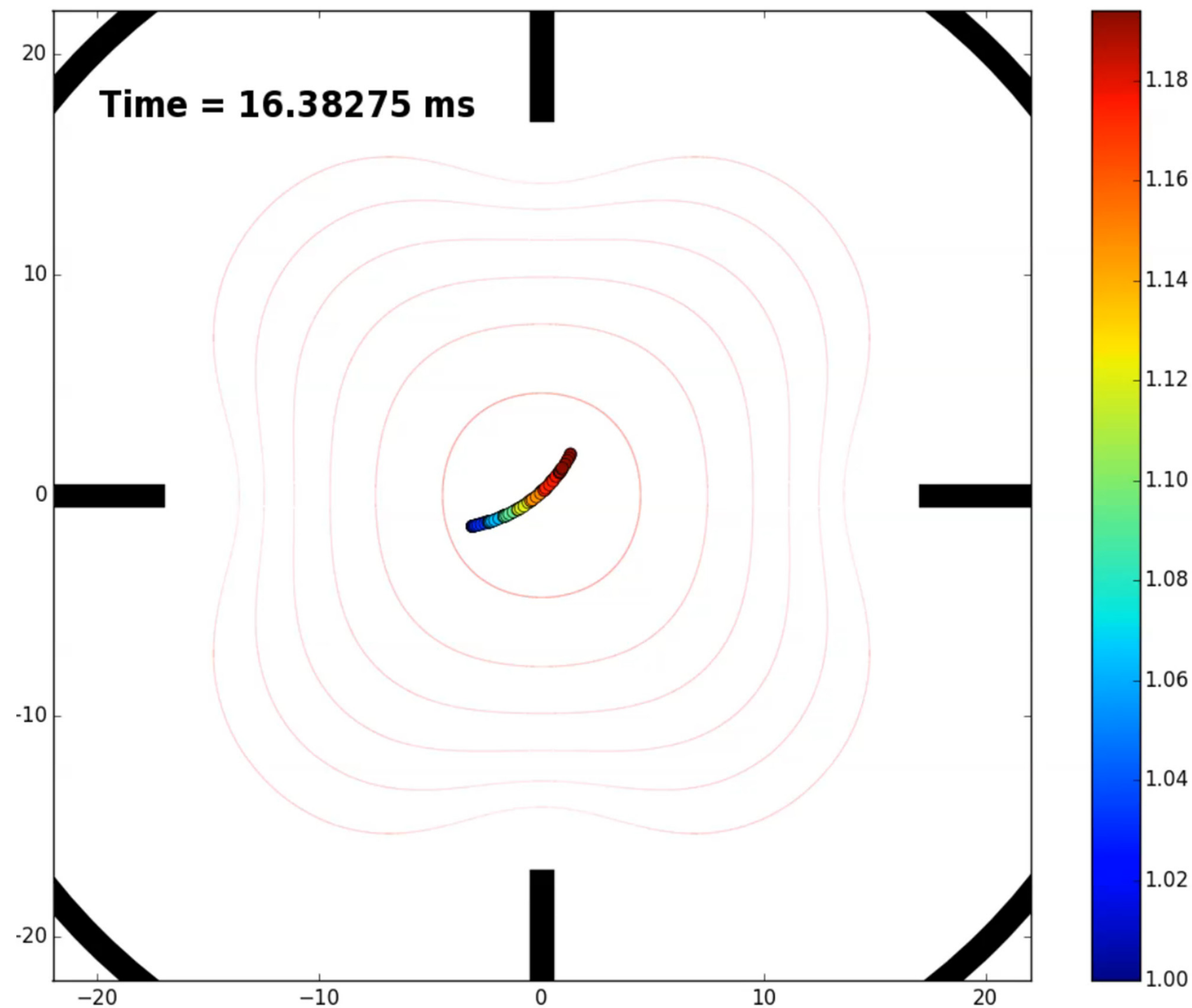
Ion excitation to a higher radius: an RF field & sidekick (**distributed ions**)

⇩

Ion detection (induced ion current)

⇩

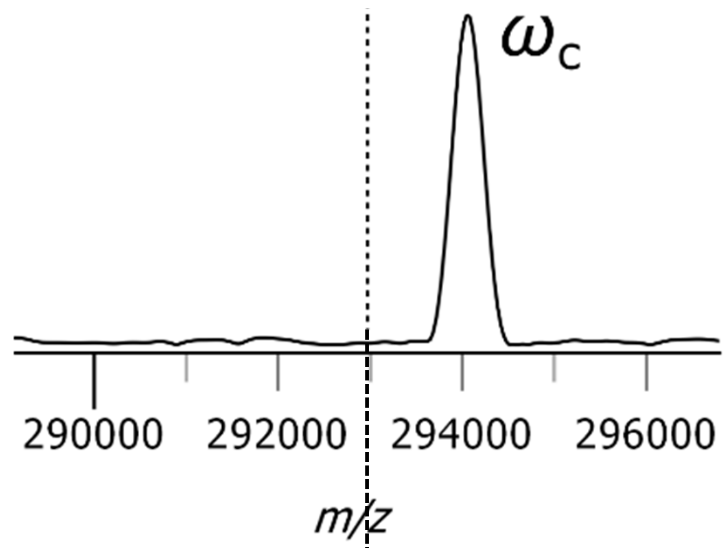
Quench of ions (ion ejection)



Nagornov et al., JASMS (2020) 31, 2258-2269

What Frequency Do We Measure?

cyclotron frequency

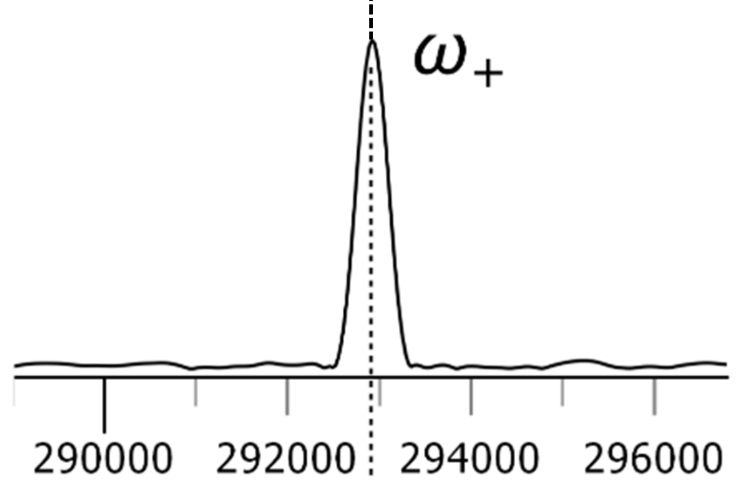


$$\omega_c = \frac{q}{m} B$$

NADEL ICR cells
distributed ions

DOI: 10.1002/mas.21681

reduced cyclotron frequency

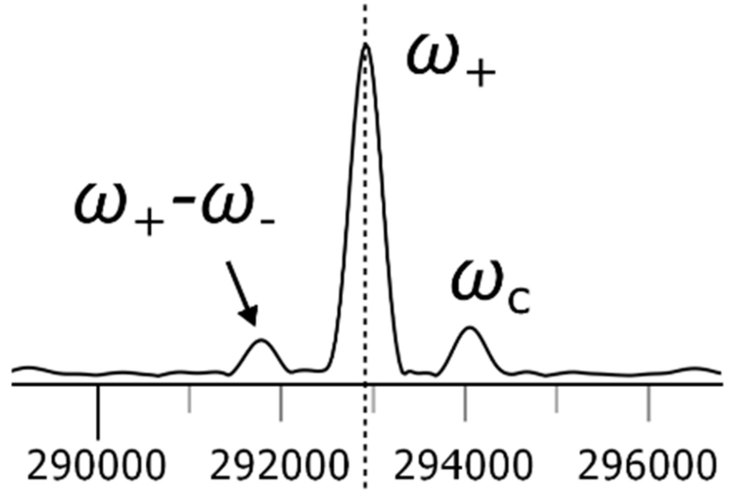


$$\omega_+ = \omega_c - \omega_-$$

magnetron (drift) frequency

Idealistic (well tuned) FT-ICR MS / MRMS

reduced cyclotron frequency (realistic case)



$$\omega_+ = \omega_c - \omega_-$$

magnetron (drift) sidebands

Conventional FT-ICR MS / MRMS
compact clouds

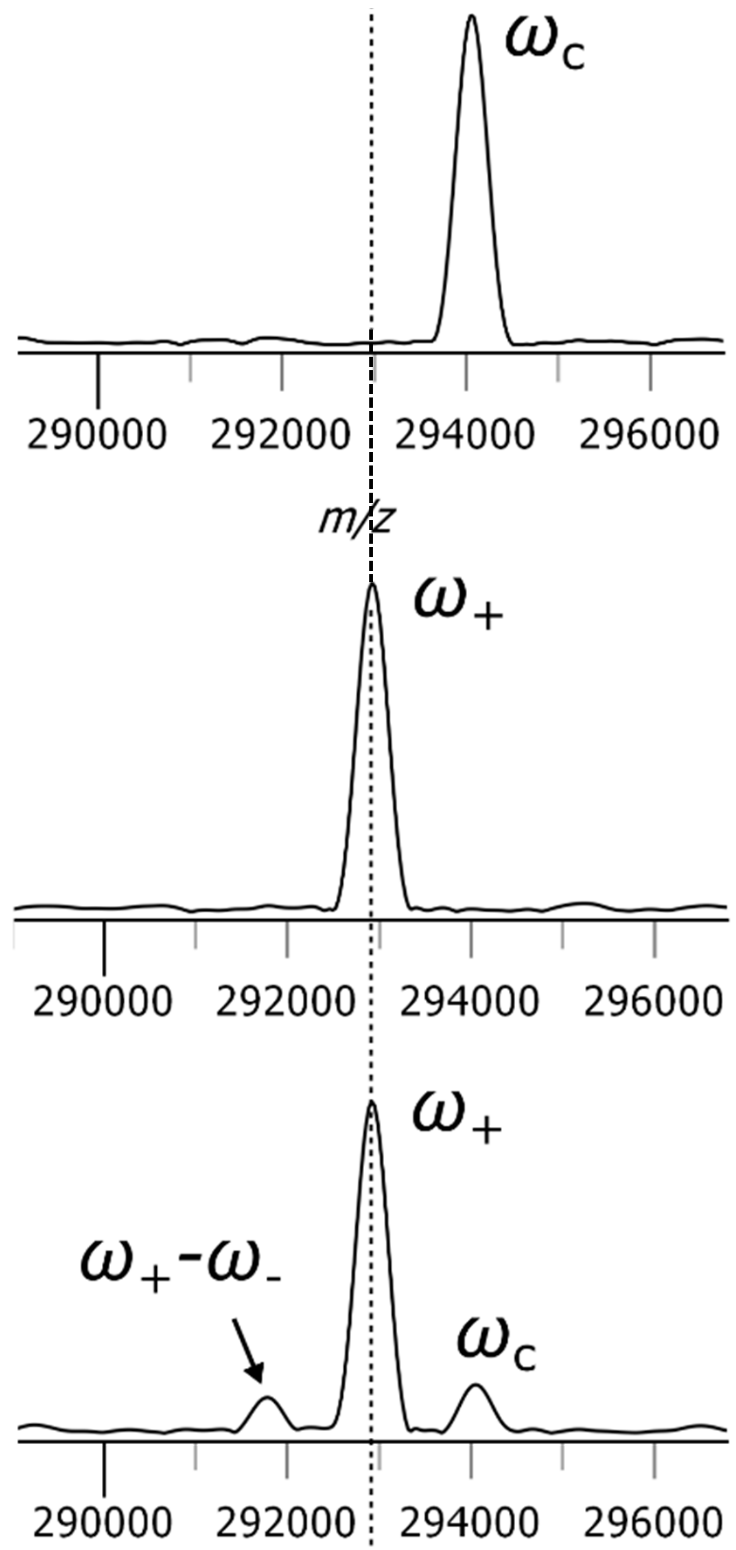
DOI: 10.1002/mas.21681

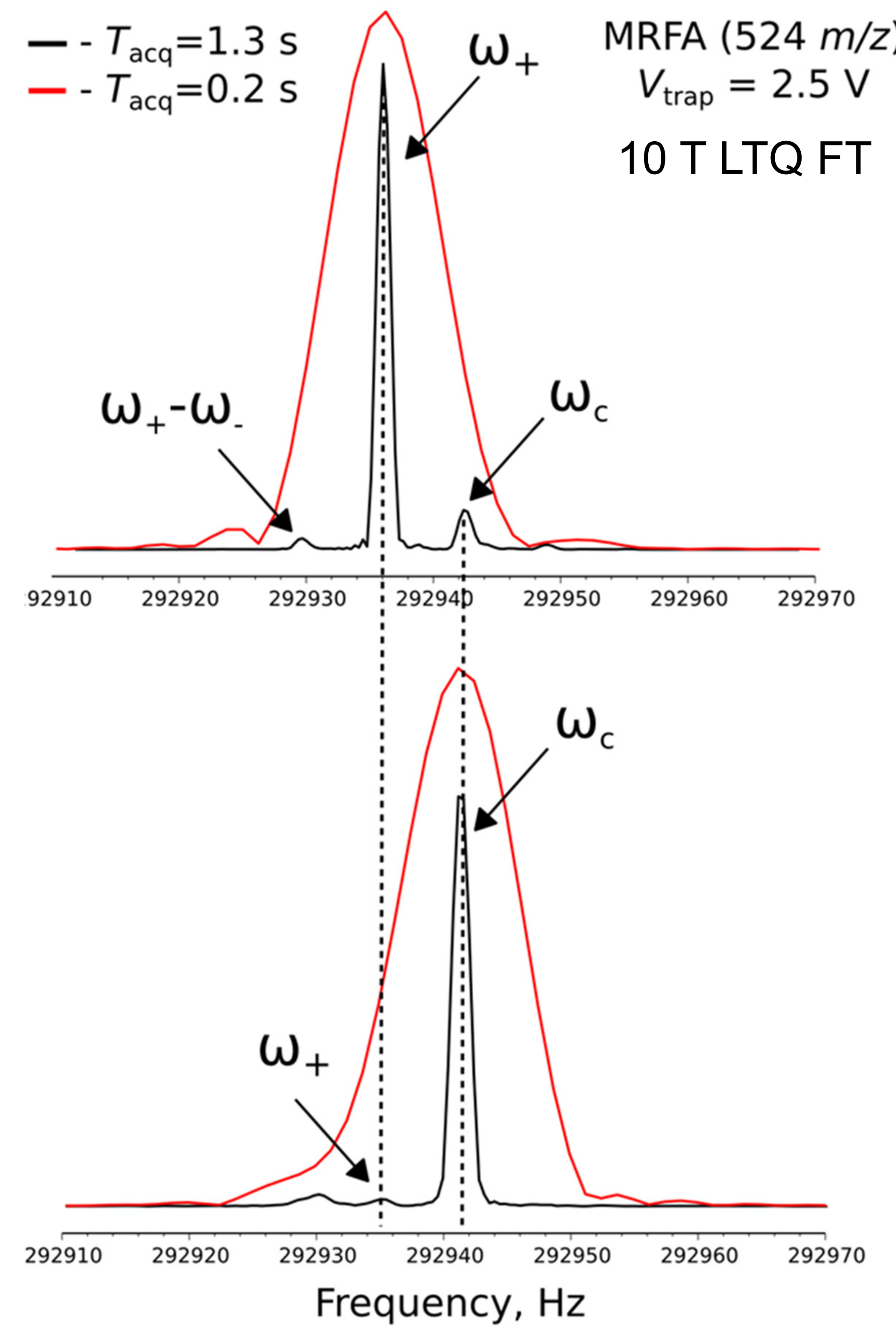
What Frequency Do We Measure?

cyclotron frequency

reduced cyclotron frequency

reduced cyclotron frequency **(realistic case)**





How Many FT-ICR MS / MRMS Are Out There?

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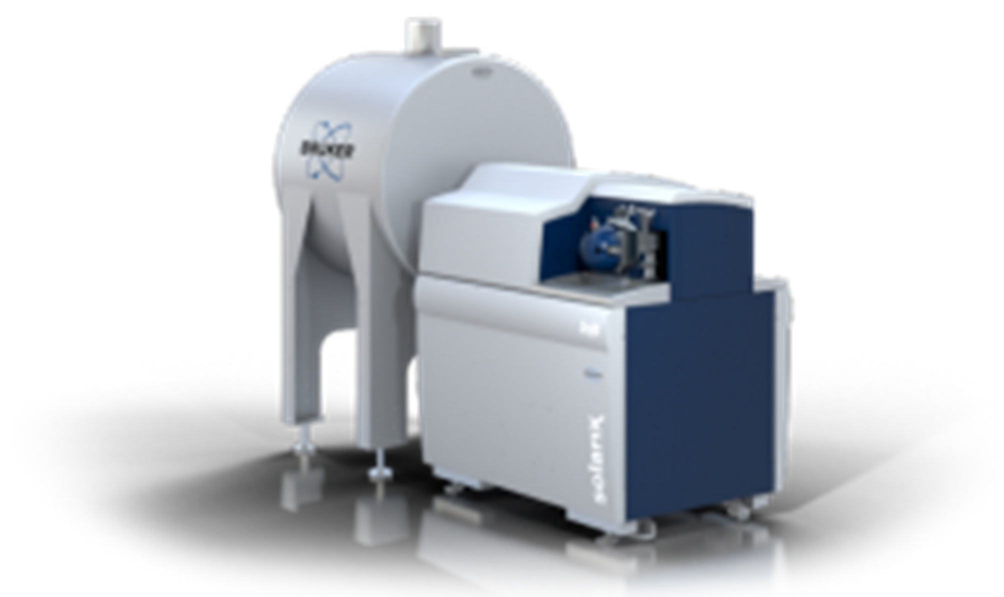
solariX MRMS

BRUKER

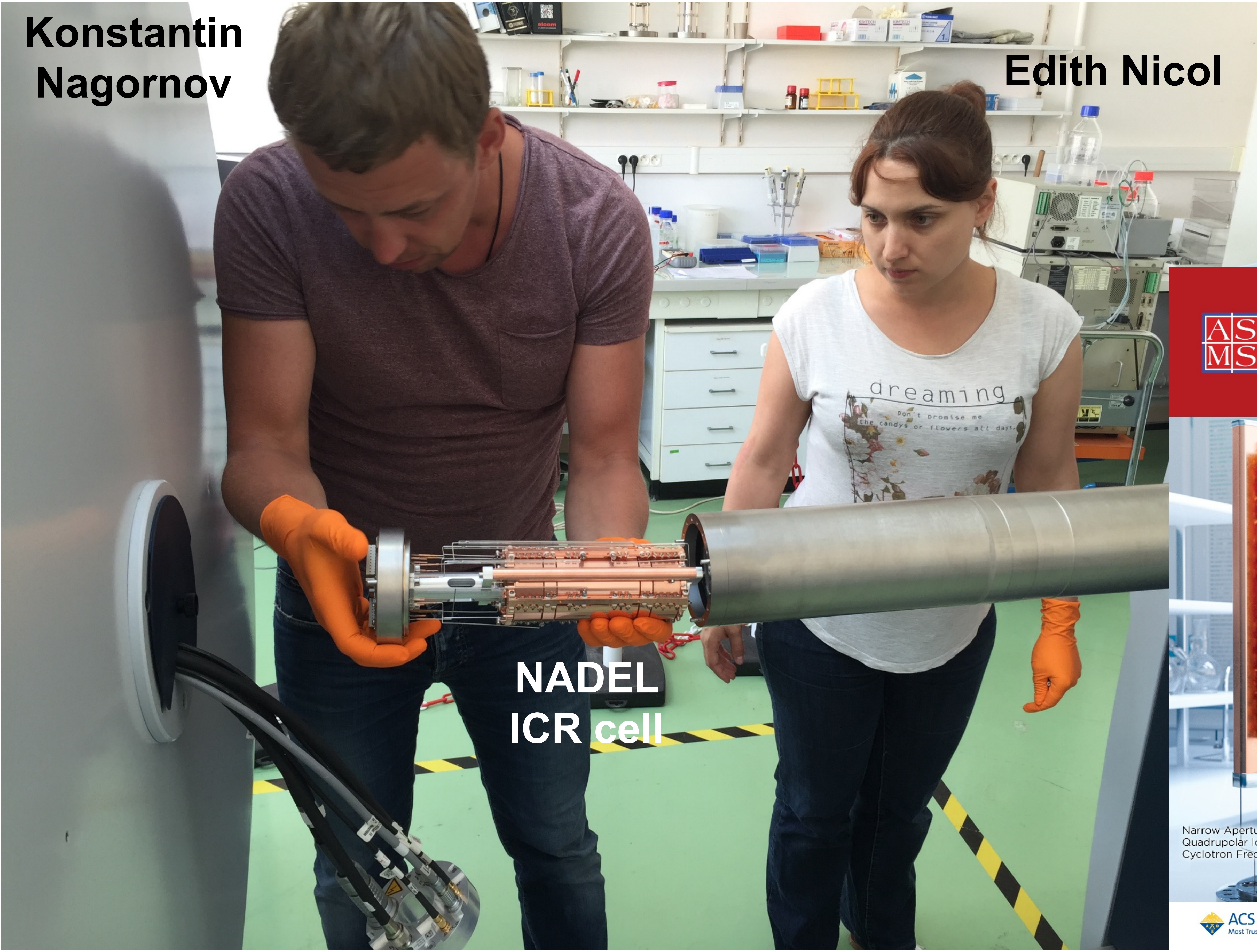
scimaX MRMS



“The workhorse platform for high-field MRMS work at 12T or 15T – useful for ultra-complex mixture analysis such as petroleomics and dissolved organic materials.”

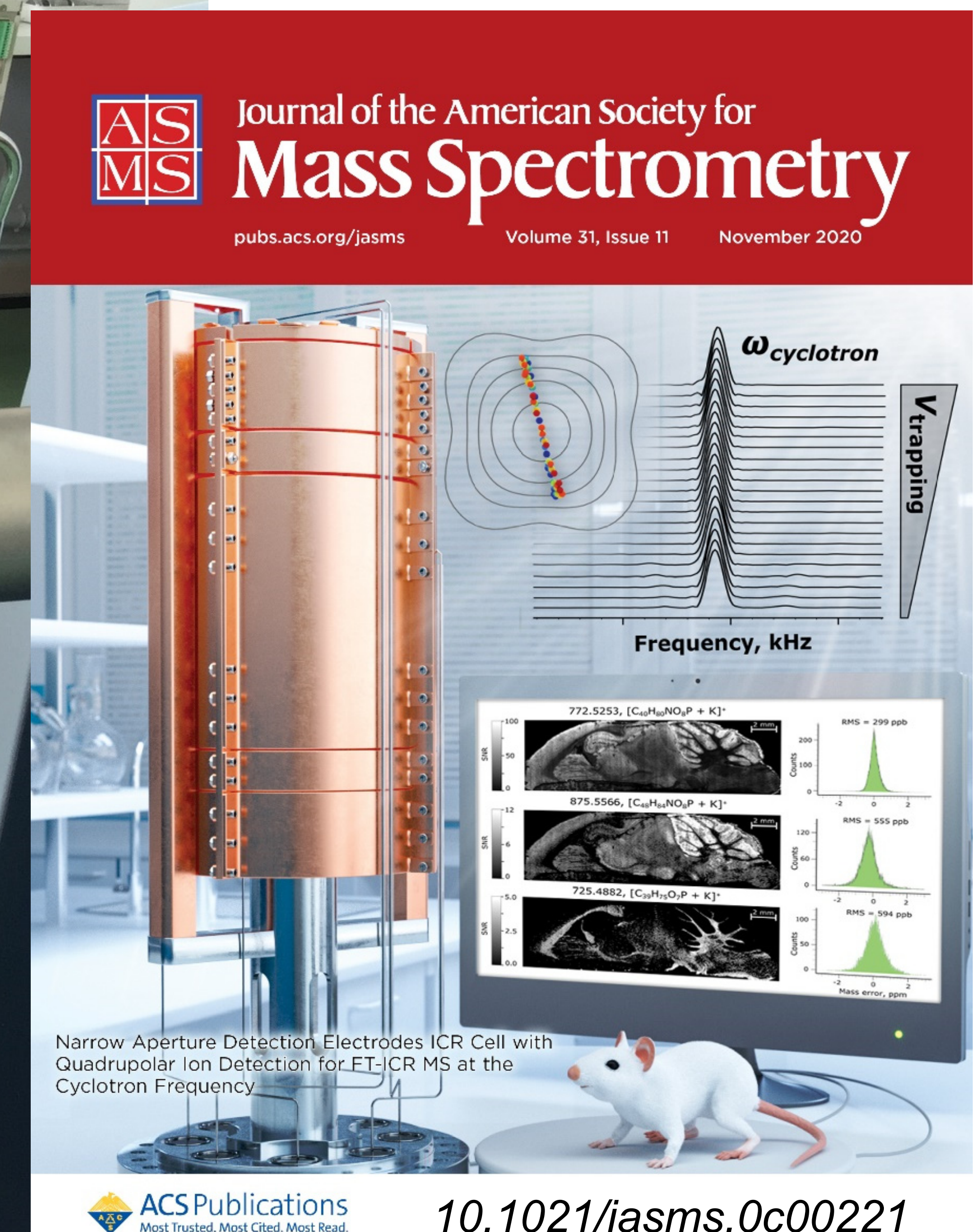
“scimaX® is powered by 2xR MRMS technology, bringing the "high hanging fruit" within easy reach”

https://www.bruker.com/en/products-and-solutions/mass-spectrometry/mrms.html

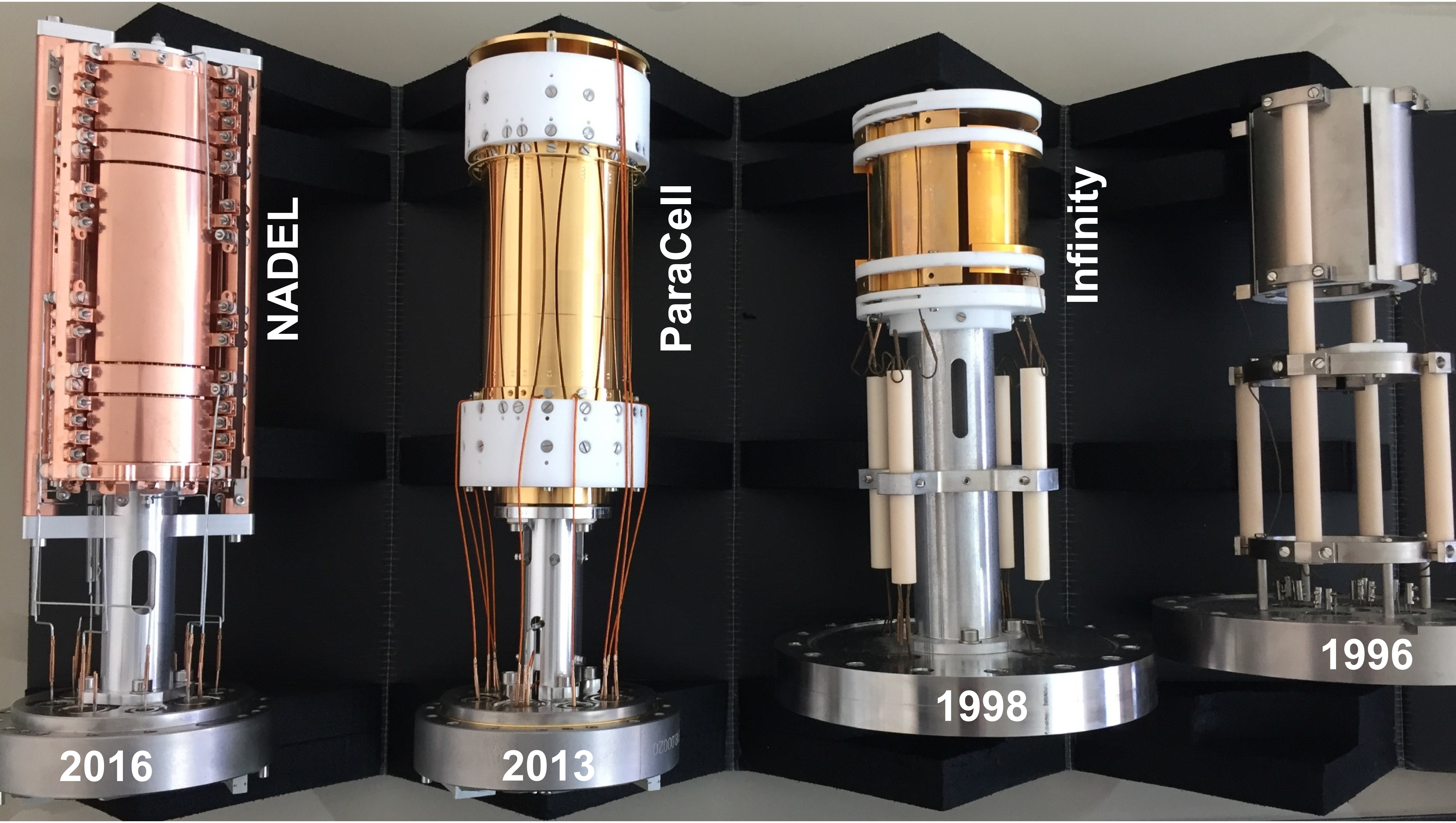


ÉCOLE POLYTECHNIQUE ParisTech

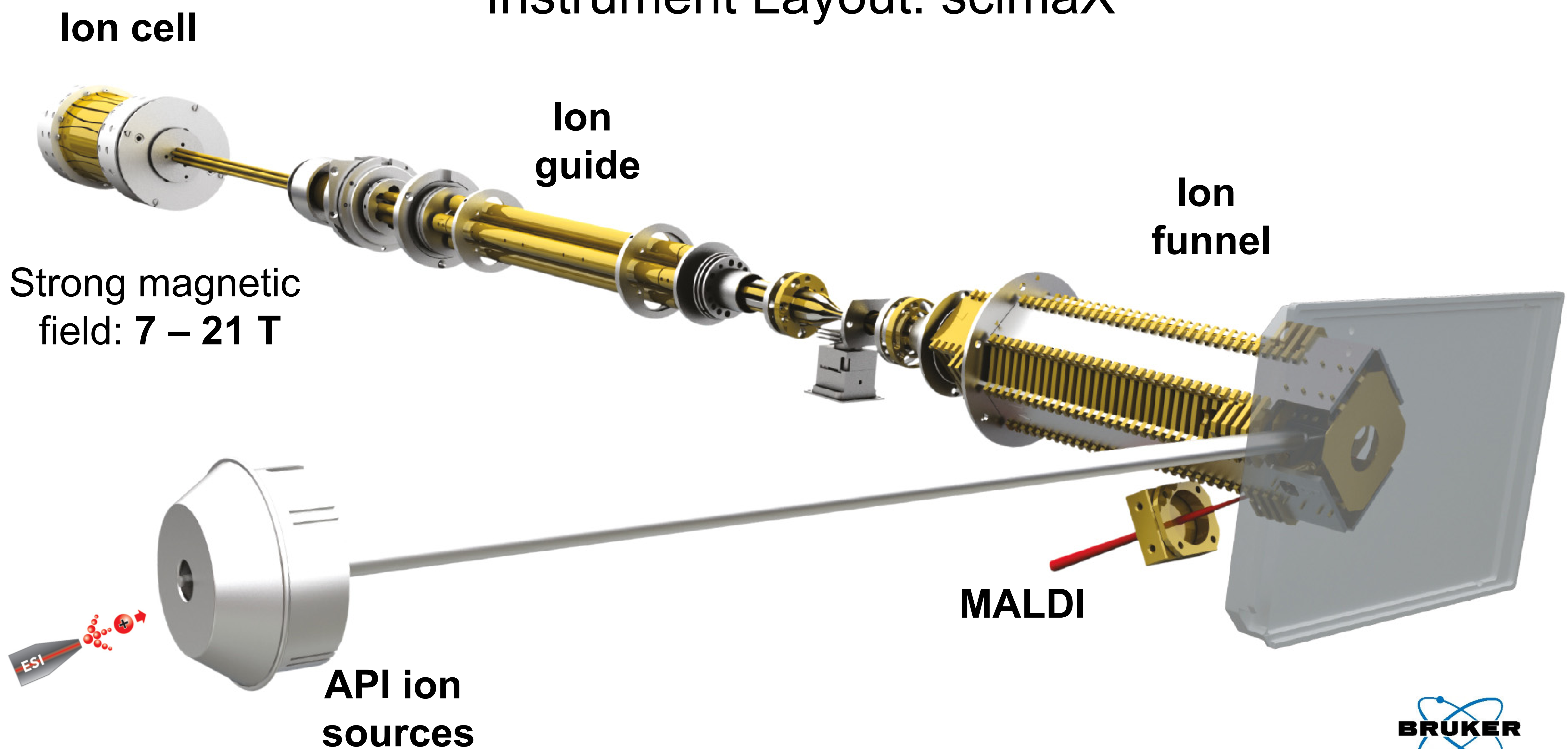
9.4 T SolariX XR



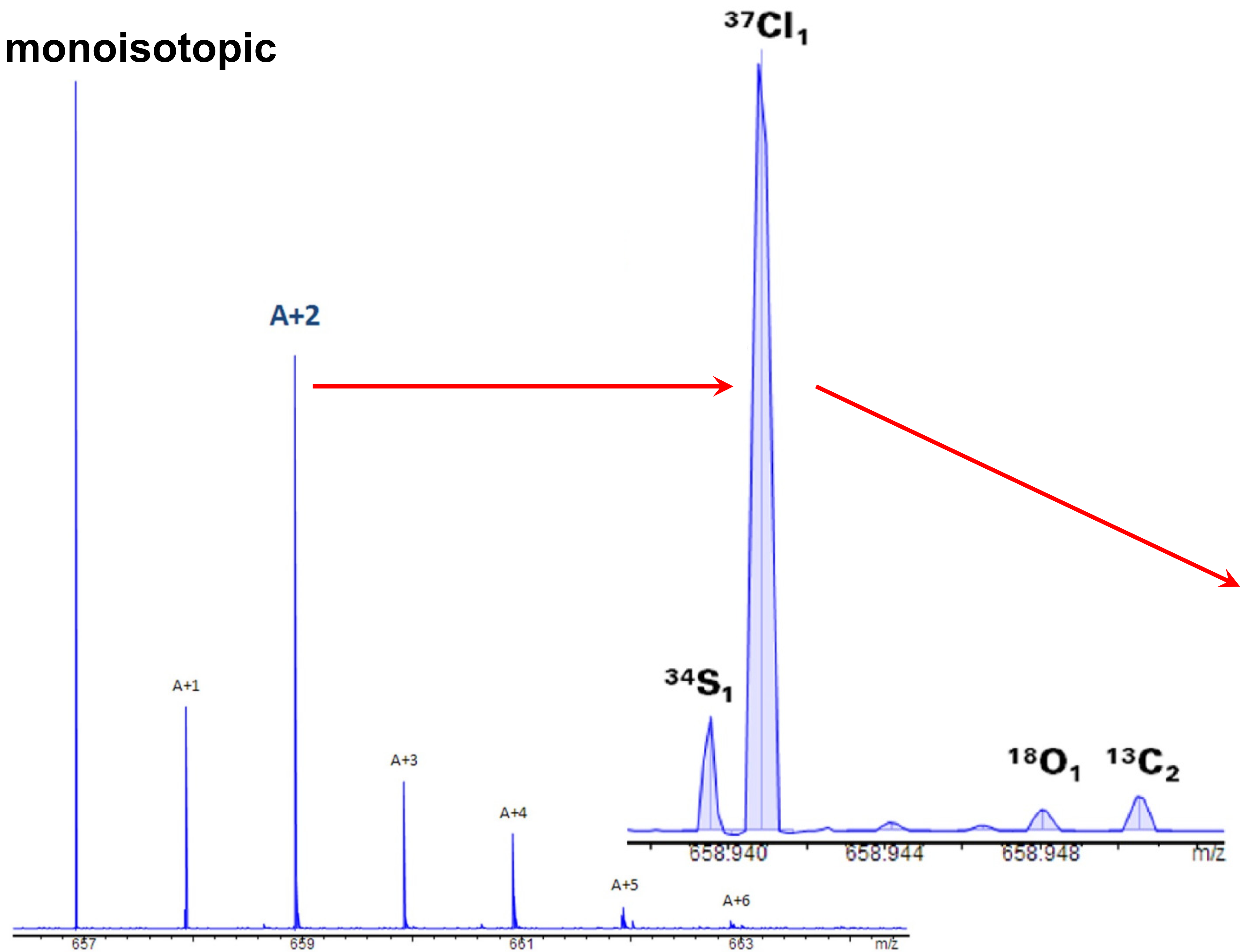
10.1021/jasms.0c00221

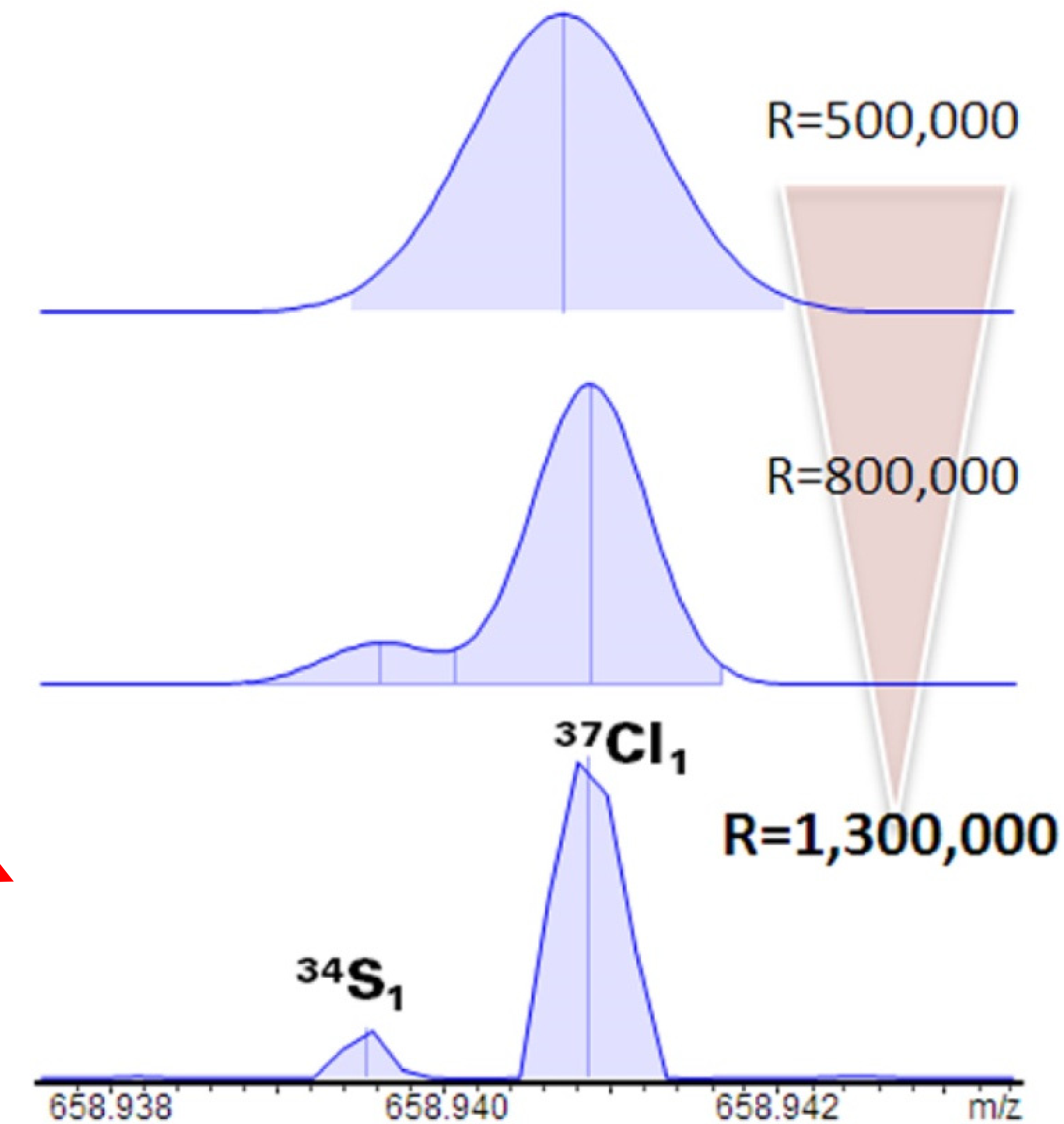

NADEL
2016
ParaCell
2013
Infinity
1998
1996

Instrument Layout: scimaX



Isotopic Fine Structure (IFS): Elemental Composition





It would require > 4.5 s transient on a Q Exactive HF – beyond commercial configuration

MRMS Instrument Specifications

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	7T solariX	12T solariX	15T solariX	7T scimaX
Maximum resolving power	>10 M	>10 M	>10 M	>20 M
Mass accuracy (internal)	600 ppb	300 ppb	250 ppb	600 ppb
ESI ion source	yes	yes	yes	yes
MALDI ion source	optional	optional	optional	yes
ETD MS/MS	optional	optional	optional	yes
Detector	ParaCell XR or 2xR	ParaCell XR	ParaCell XR	ParaCell 2xR
Magnetic field	7 T	12 T	15 T	7 T cc
Annual cryogen fill	yes	yes	yes	no
Quench line required	yes	yes	yes	no

- 2xR: ion detection at the second **frequency multiple** (double frequency)
- “cc” magnet: “cryogen-free” magnet

Bruce et al., IJMS (2021) DOI: 10.1016/j.ijms.2021.116578

Nagornov et al., Anal. Chem. (2014) 86, 18, 9020-9028

NATIONAL HIGH MAGNETIC FIELD LABORATORY

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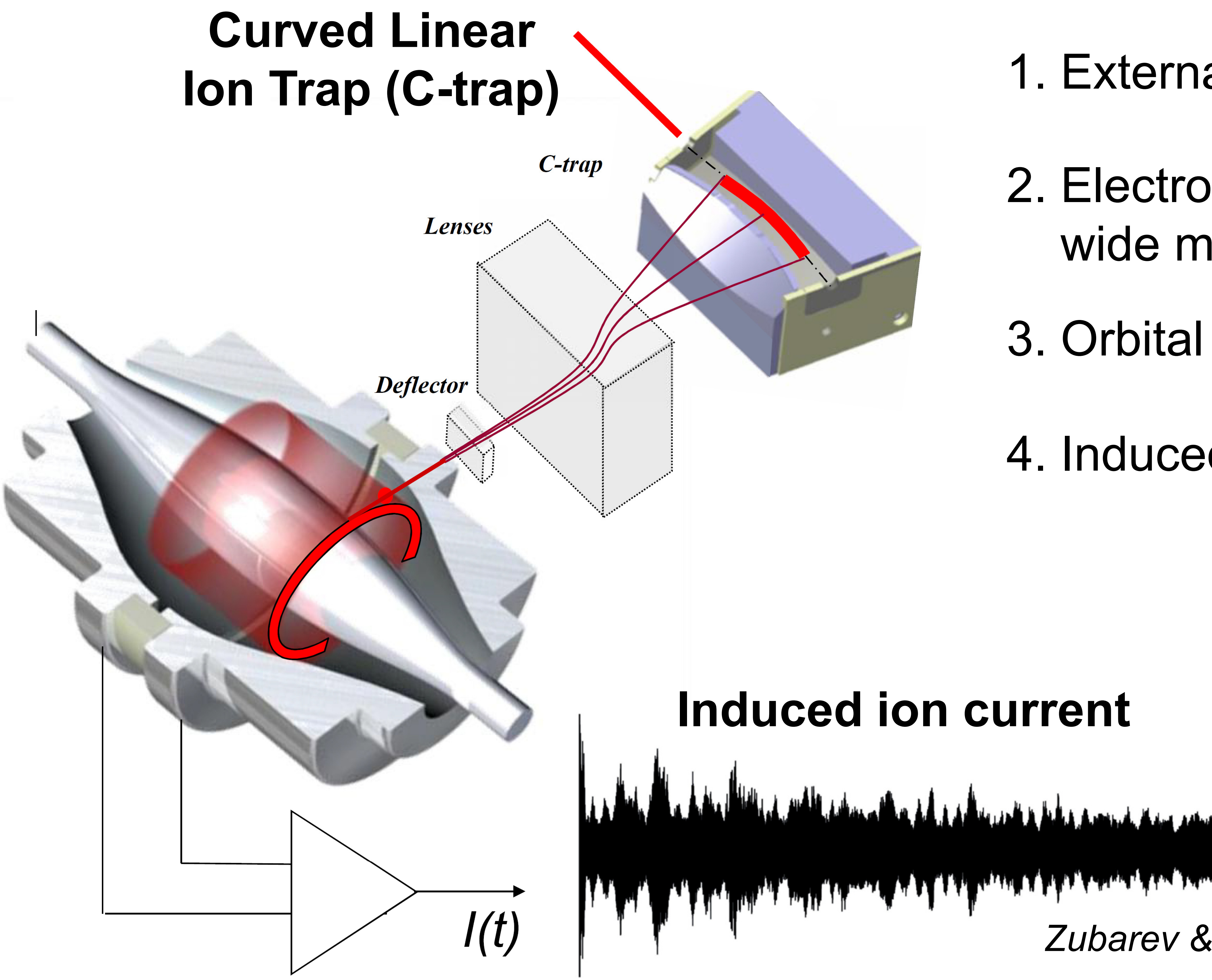
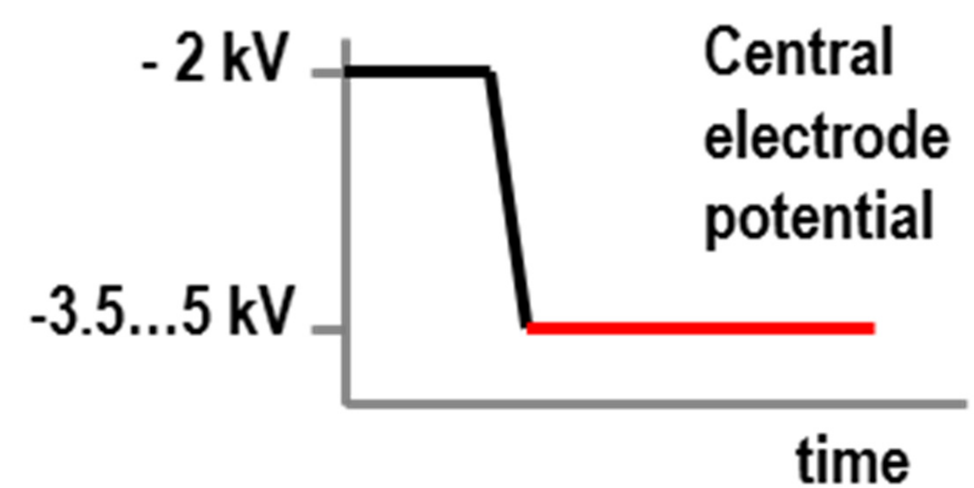
Orbitrap Mass Analyzer and C-Trap: Solo or Duet?



1. External pulsed ion source
2. Electrodynamic squeezing: wide mass (*m/z*) range
3. Orbital trapping and oscillations
4. Induced ion current detection



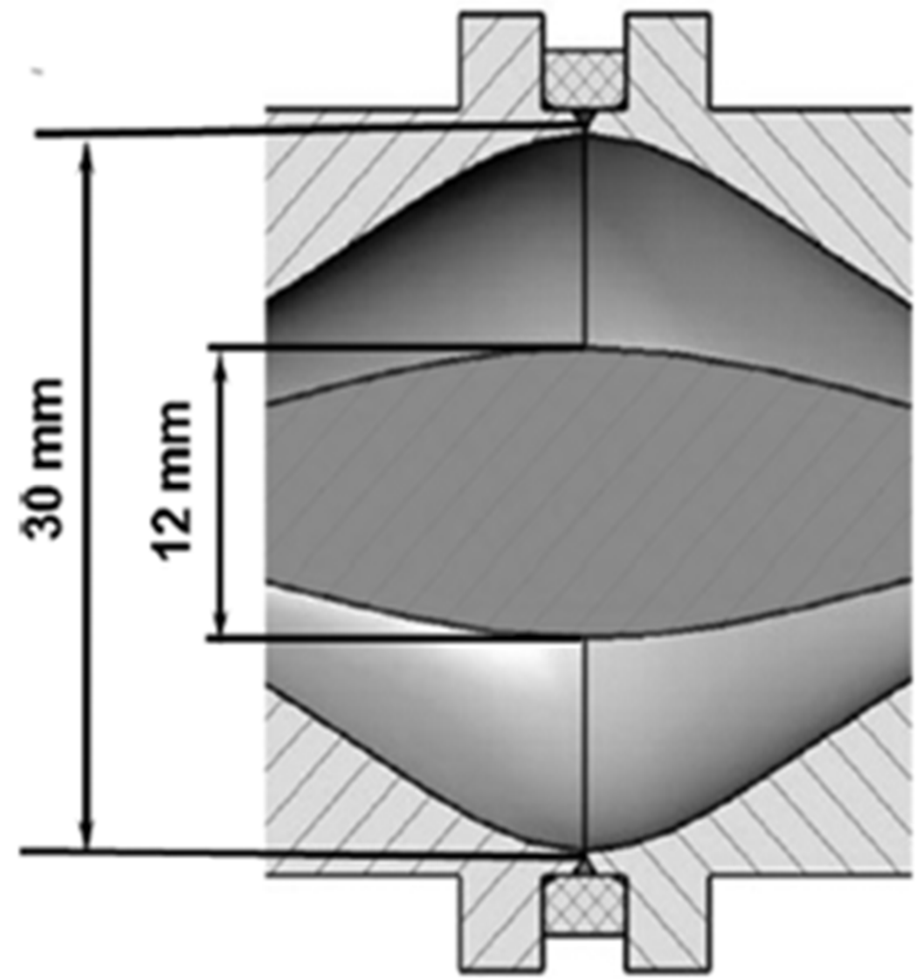
Zubarev & Makarov., Anal. Chem. (2013) 85, 5288

The Two Orbitrap Models: **D30** and **D20**

Alexander Makarov

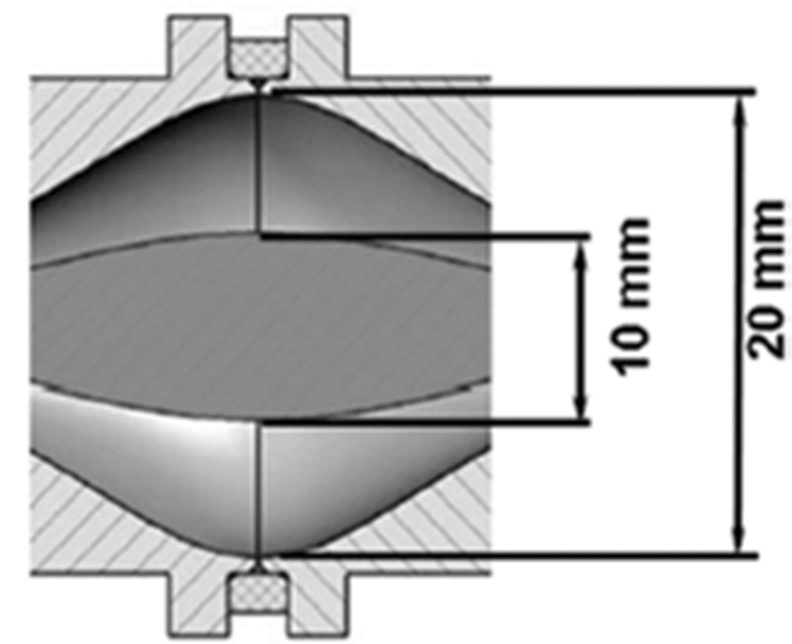
Makarov, Anal. Chem. (2000) 72, 1156

D30 Orbitrap (Regular)



3.5 kV; 5 kV

D20 Orbitrap (Compact)



3.5 kV; 4 kV; 5 kV

Makarov et al., JASMS, (2009) 20, 1391-1396

Ion Oscillation Frequency in Orbitraps

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$$f = \frac{1}{2\pi}\omega = \frac{1}{2\pi}\sqrt{\frac{e/u}{(m/z)} \cdot \frac{2\cdot[V]}{R_m^2 \cdot ln\left(\frac{R_2}{R_1}\right) - \frac{1}{2}[R_2^2 - R_1^2]}}$$

where e is the elementary charge, u is the unified atomic mass unit, V is the central electrode voltage, R_1 and R_2 are the circumscribed radius of the central electrode and the inscribed radius of the outer electrode in the central plane, respectively. The R_m is the characteristic radius, which is usually set close to $R_m = R_2\sqrt{2}$ in order to meet the ion trapping condition. For the regular, D30, Orbitrap geometry: $R_1 = 6\ mm$, $R_2 = 15\ mm$, $R_m = 21.2\ mm$, and thus $ln\left(\frac{R_2}{R_1}\right) = 0.91$. Corresponding scaling down in size for the compact, D20, Orbitrap results in the following parameters: $R_1 = 5\ mm$, $R_2 = 10\ mm$, $R_m = 14.1\ mm$, and thus $ln\left(\frac{R_2}{R_1}\right) = 0.69$.

- What is *k*? $\omega \approx \sqrt{\frac{k}{m/z}}$

Makarov, A., Denisov, E., Lange, O., *JASMS*, 20 (2009) 1391-1396

Tsybin *et al. “Advanced FTMS Fundamentals”, Chapter 5*

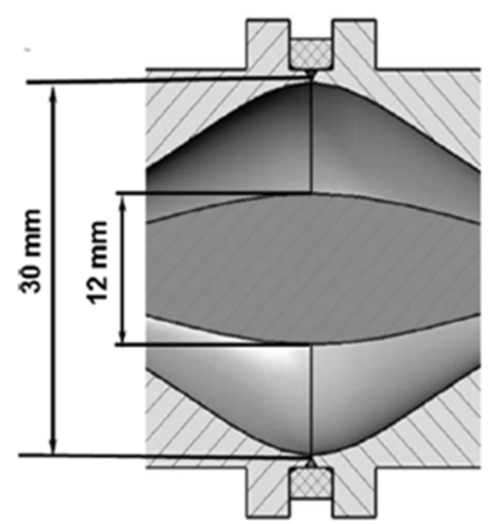
Regular (D30) vs. Compact (D20) Orbitrap

For signals at the equal frequencies:

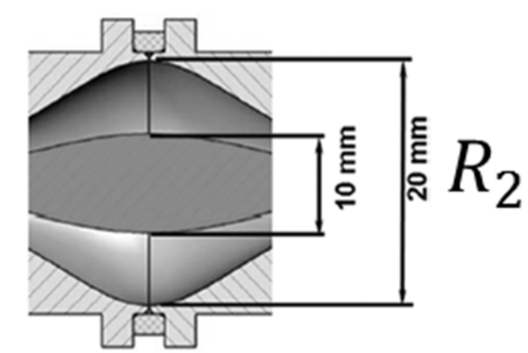
$$\frac{(m/z)_{D20}}{(m/z)_{D30}} = \frac{\left(R_m^2 \cdot ln\left(\frac{R_2}{R_1}\right) - \frac{1}{2}\left[R_2^2 - R_1^2\right]\right)_{D30}}{\left(R_m^2 \cdot ln\left(\frac{R_2}{R_1}\right) - \frac{1}{2}\left[R_2^2 - R_1^2\right]\right)_{D20}} = 3.1$$

$$R_m = R_2\sqrt{2}$$

D30 Orbitrap



D20 Orbitrap



Makarov, A., Denisov, E., Lange, O., *JASMS*, 20 (2009) 1391-1396
Tsybin *et al. "Advanced FTMS Fundamentals", Chapter 5*

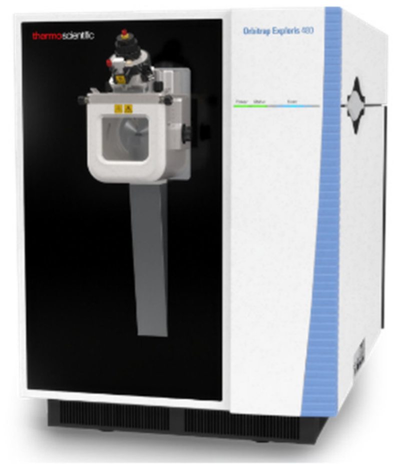
Orbitrap Technology Concepts

1. Ion Excitation by Injection (electrodynamic squeezing)
2. Maximum injection time (**ITmax**)
3. Automatic Gain Control (**AGC**)
4. Normalized level (**NL**)
5. Enhanced Fourier transform (**eFT**)
6. Parallel ion detection and accumulation/fragmentation
7. Microscans: transient averaging
8. Scans: spectral averaging
9. Mass spectra: full & reduced profile, centroids

Spectroswiss

How Many Orbitraps Are Out There?

Exploris 480



Lumos

Exploris 240

ThermoFisher SCIENTIFIC

Q Exactive
Q Exactive HF

LTQ Orbitrap XL
LTQ Orbitrap Velos
LTQ Orbitrap Elite

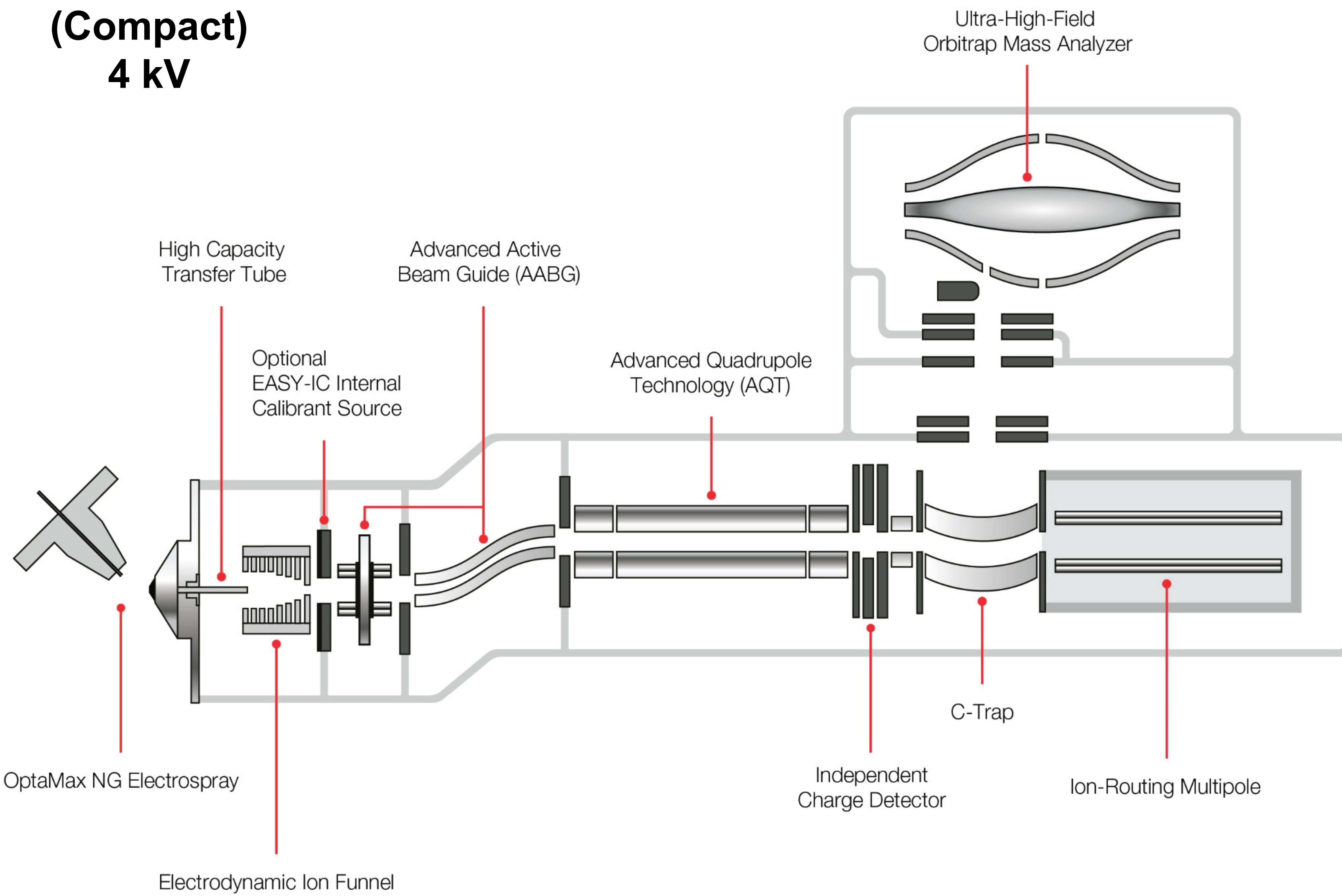
Exploris 120

Eclipse

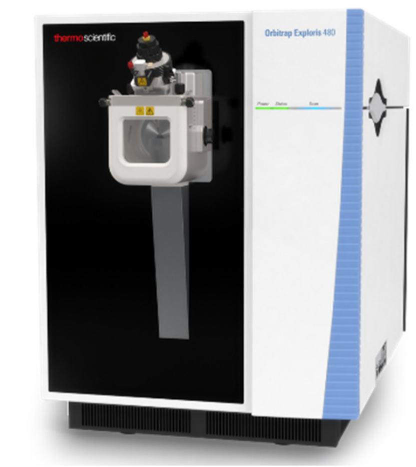
Orbitrap Models: **D30** and **D20**

Hybrid Orbitrap: **Exploris**

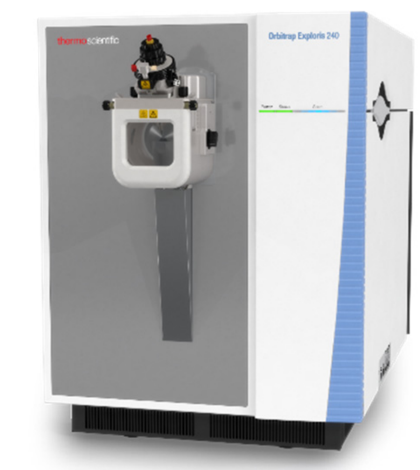
D20 Orbitrap (Compact) 4 kV



480



240

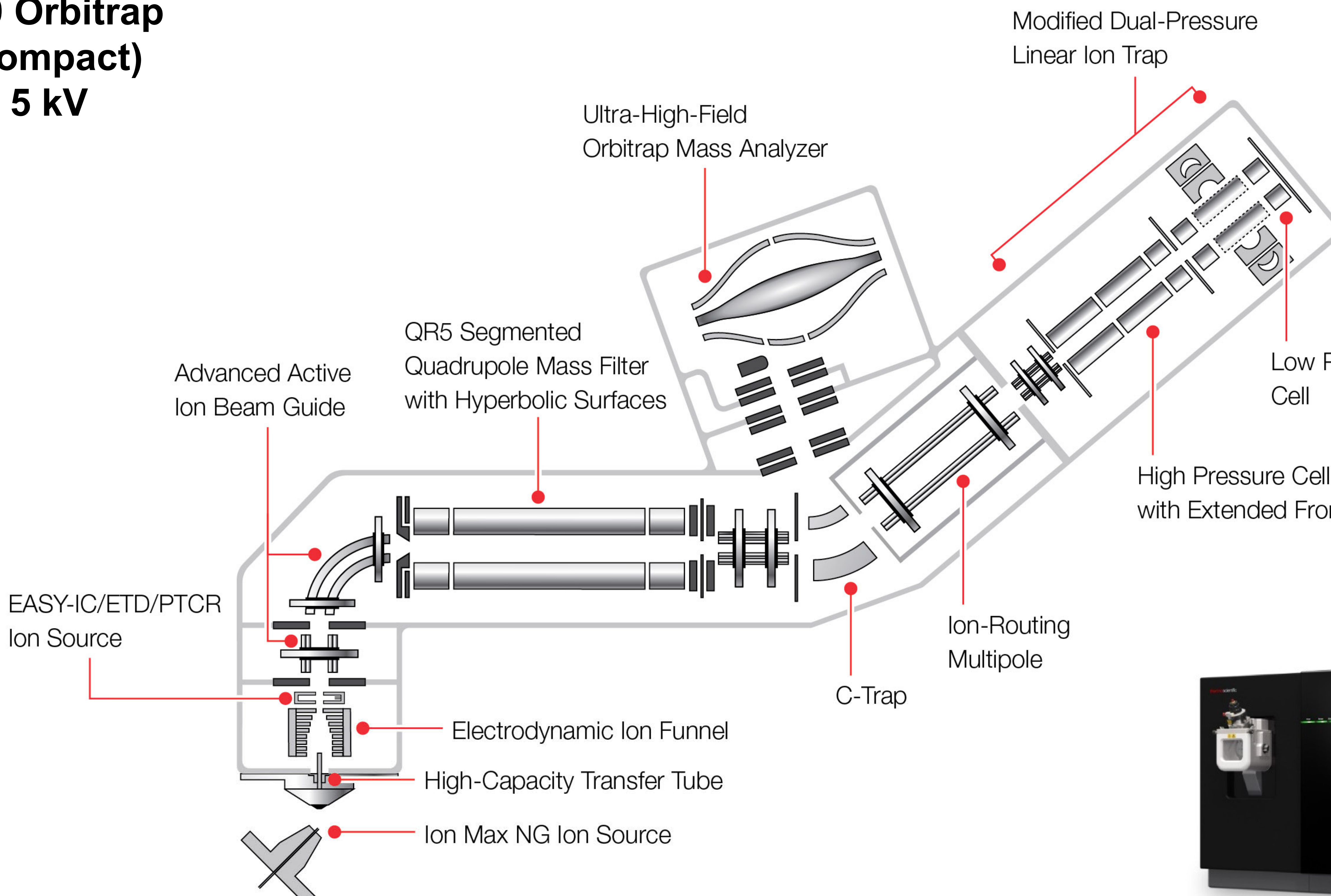


120

Spectroswiss

Tribrid Orbitrap: **Eclipse**

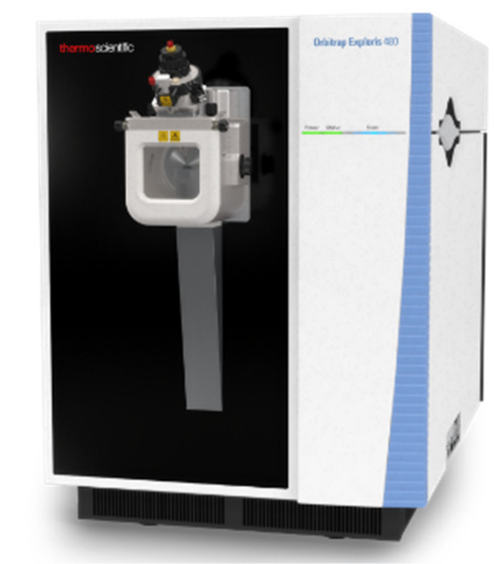
D20 Orbitrap
(Compact)
5 kV



Spectroswiss

Orbitrap Figures of Merit: 2021

Analytical Characteristic	Orbitrap Model	
	Exploris 480 (QE)	**Eclipse (Fusion)**
Mass range	*m/z* **40**-6000	*m/z* 50-2000
Frequencies	2 MHz – 168 kHz	2 MHz – 325 kHz
Spindel potential	4 kV	5 kV
Extended range	up to 8000 *m/z* with BioPharma option	
Resolution	7500 to 480,000 (500,000) at *m/z* 200	
Transients	from 16 ms to 1 second	
Ultra-high Res	(with external DAQ)	1 million @ *m/z* 200
Scan speed	up to **40 Hz** at resolution 7500 at *m/z* 200	
Dynamic range	**>5000** within a single OT mass spectrum	
Mass accuracy	**<3 ppm** RMS using **external calibration** **<1 ppm** RMS using **internal calibration**	



FTMS: Fundamentals and Data Processing

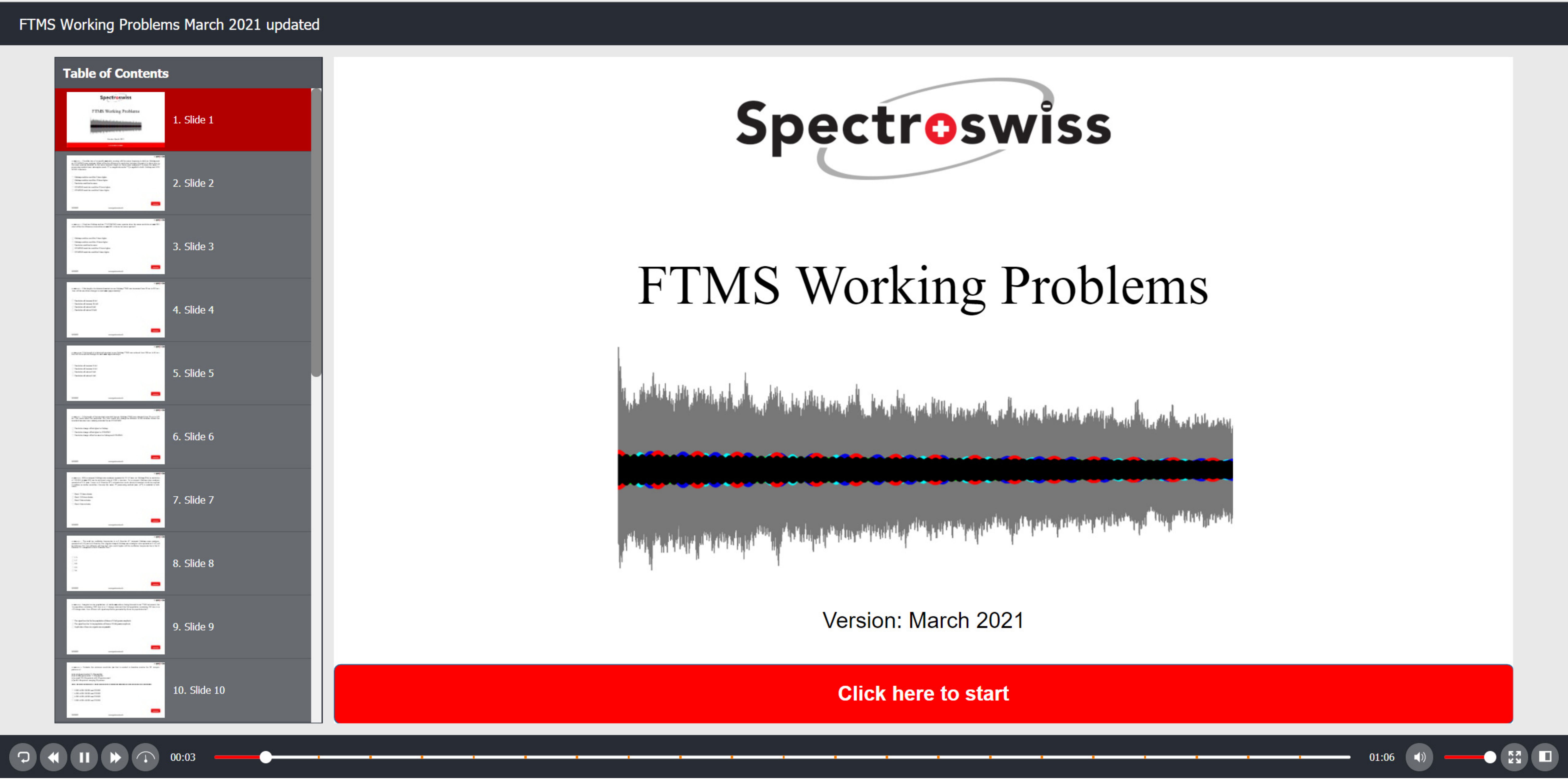
I. FTMS Fundamentals: General

II. FT-ICR MS / MRMS: Principles of Operation

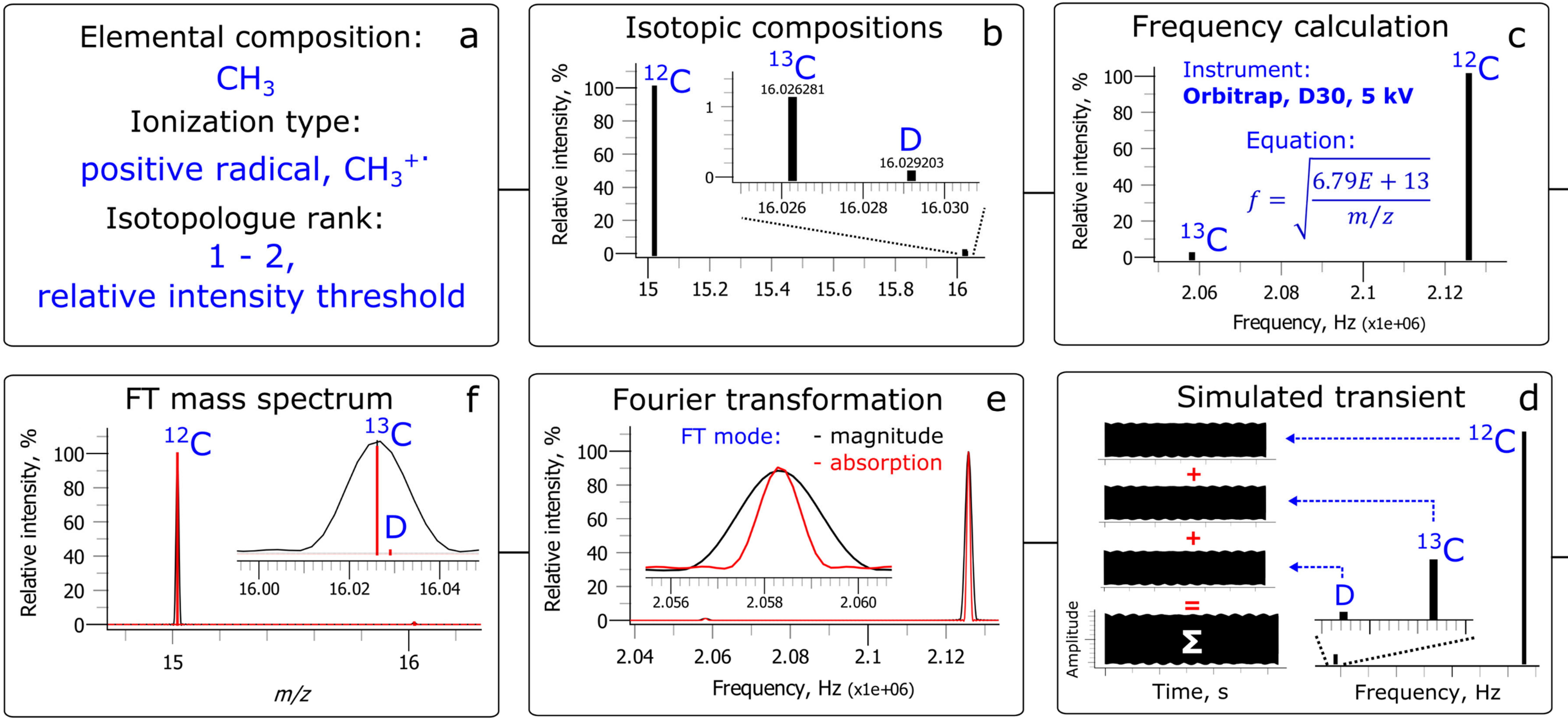
III. Orbitrap FTMS: Principles of Operation

IV. FTMS Data Processing

FTMS Quiz: http://spectroswiss.ch/quiz/

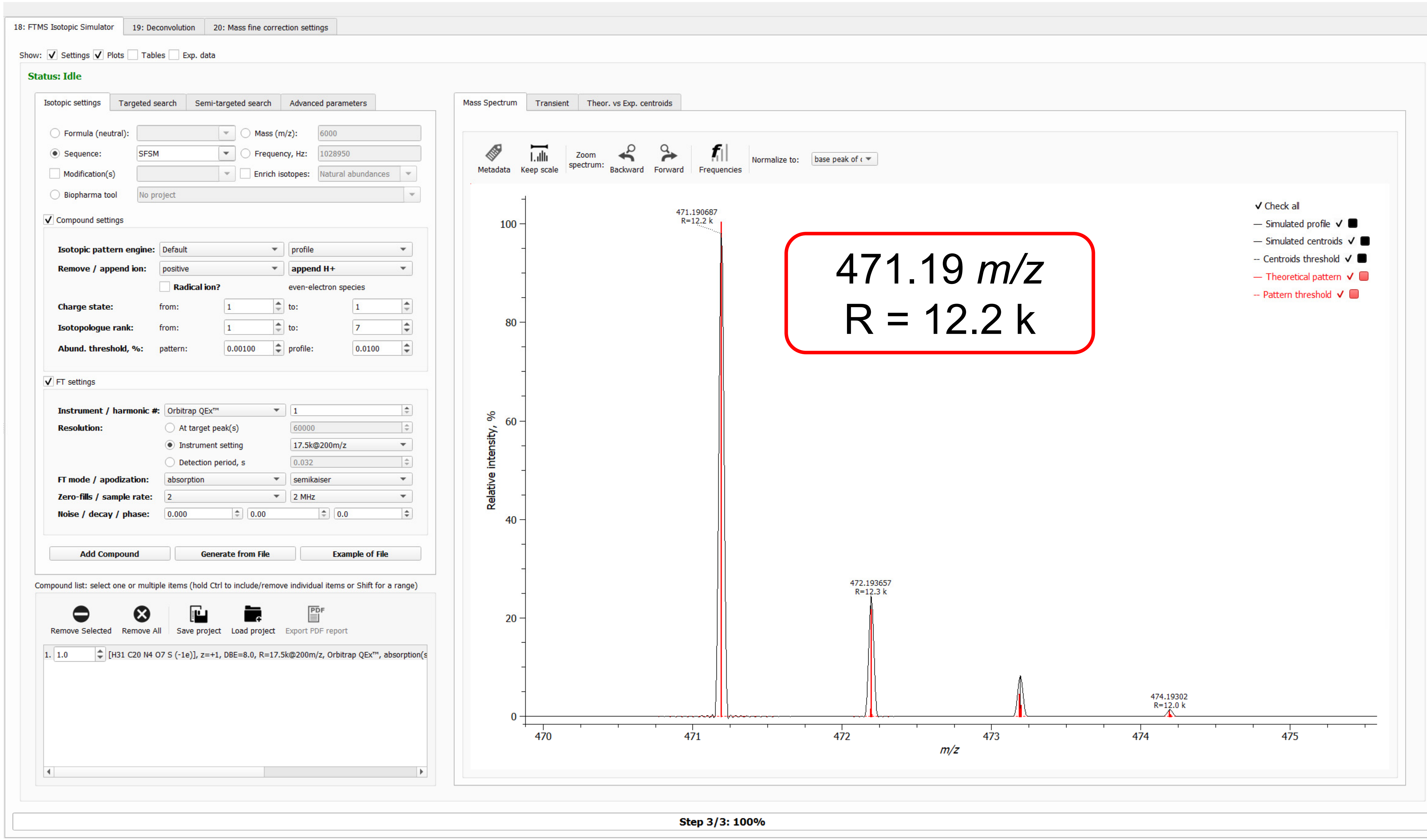


FTMS Data Processing: Step by Step

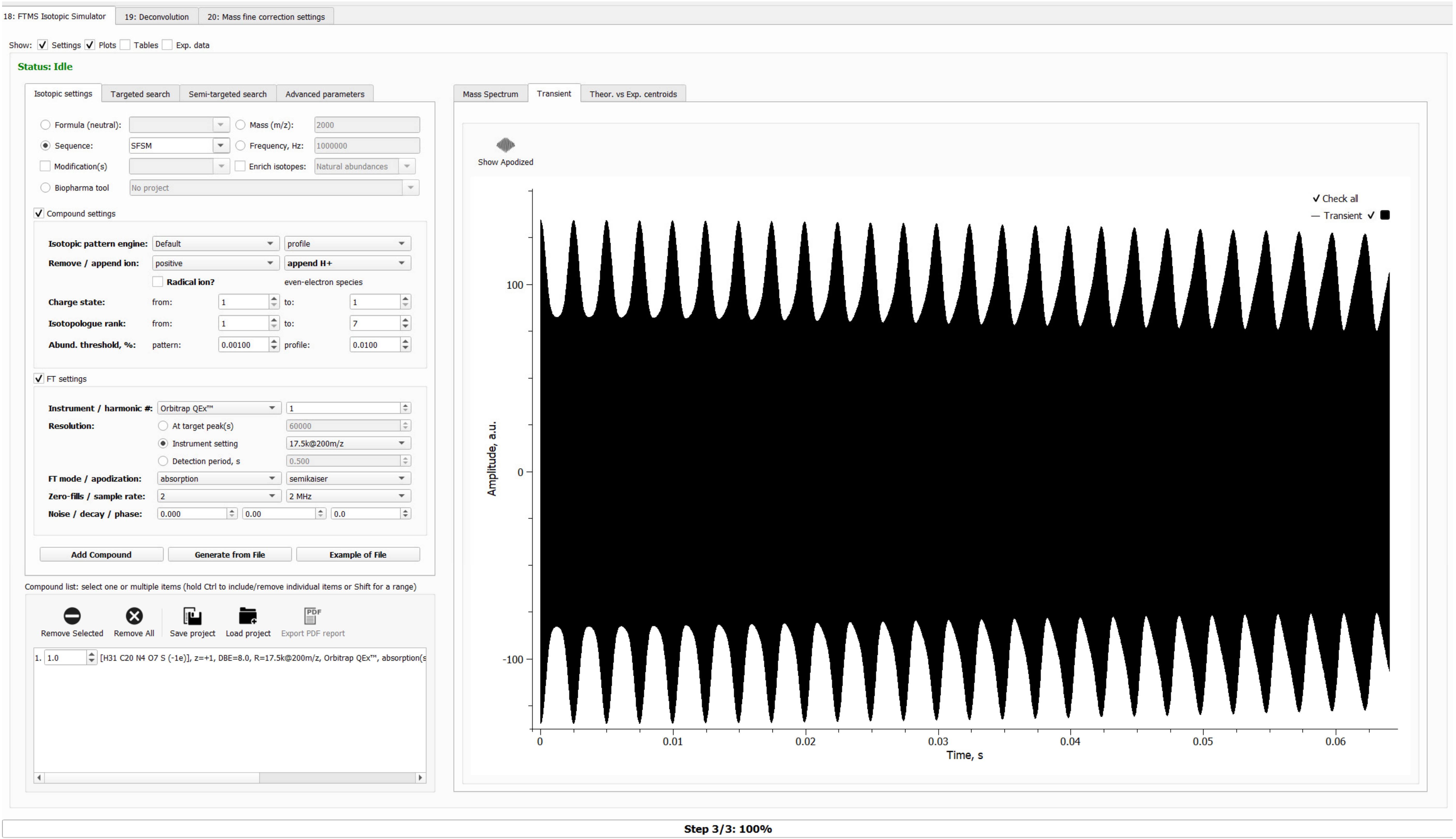


DOI: 10.1021/jasms.0c00190

FTMS Isotopic Simulator: SFSM Peptide Analysis



SFSM peptide analysis with FTMS: **transient**



64 ms

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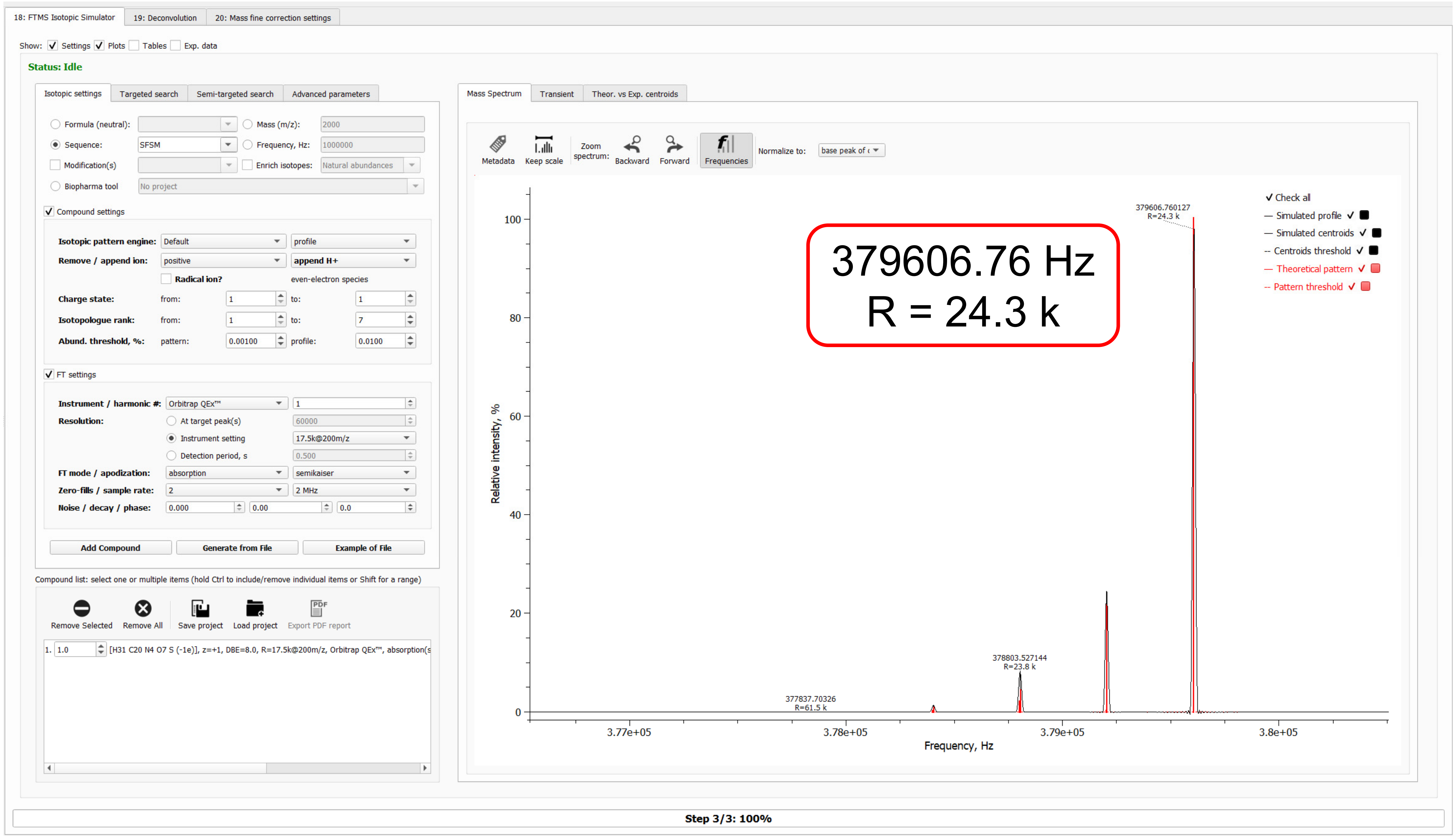
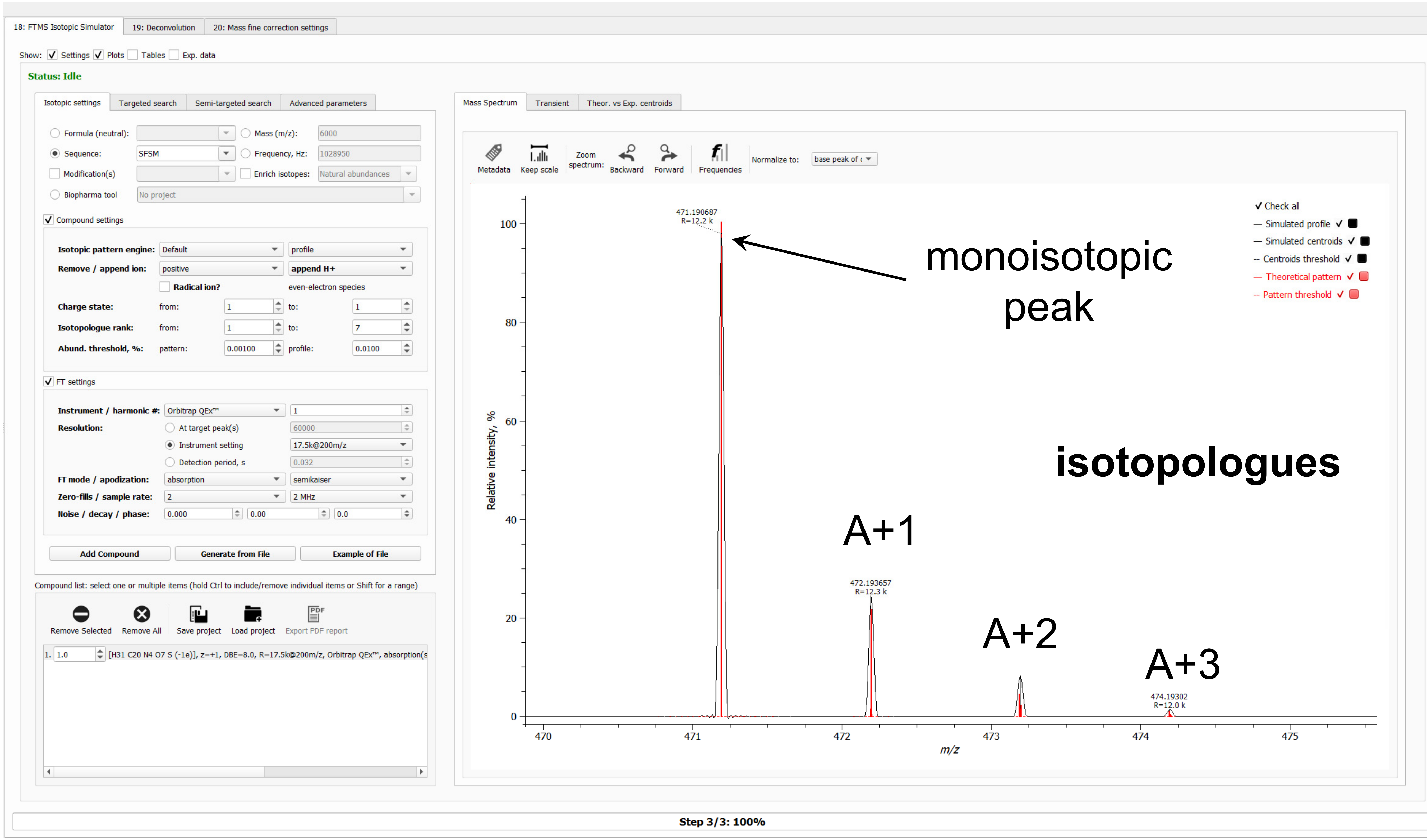
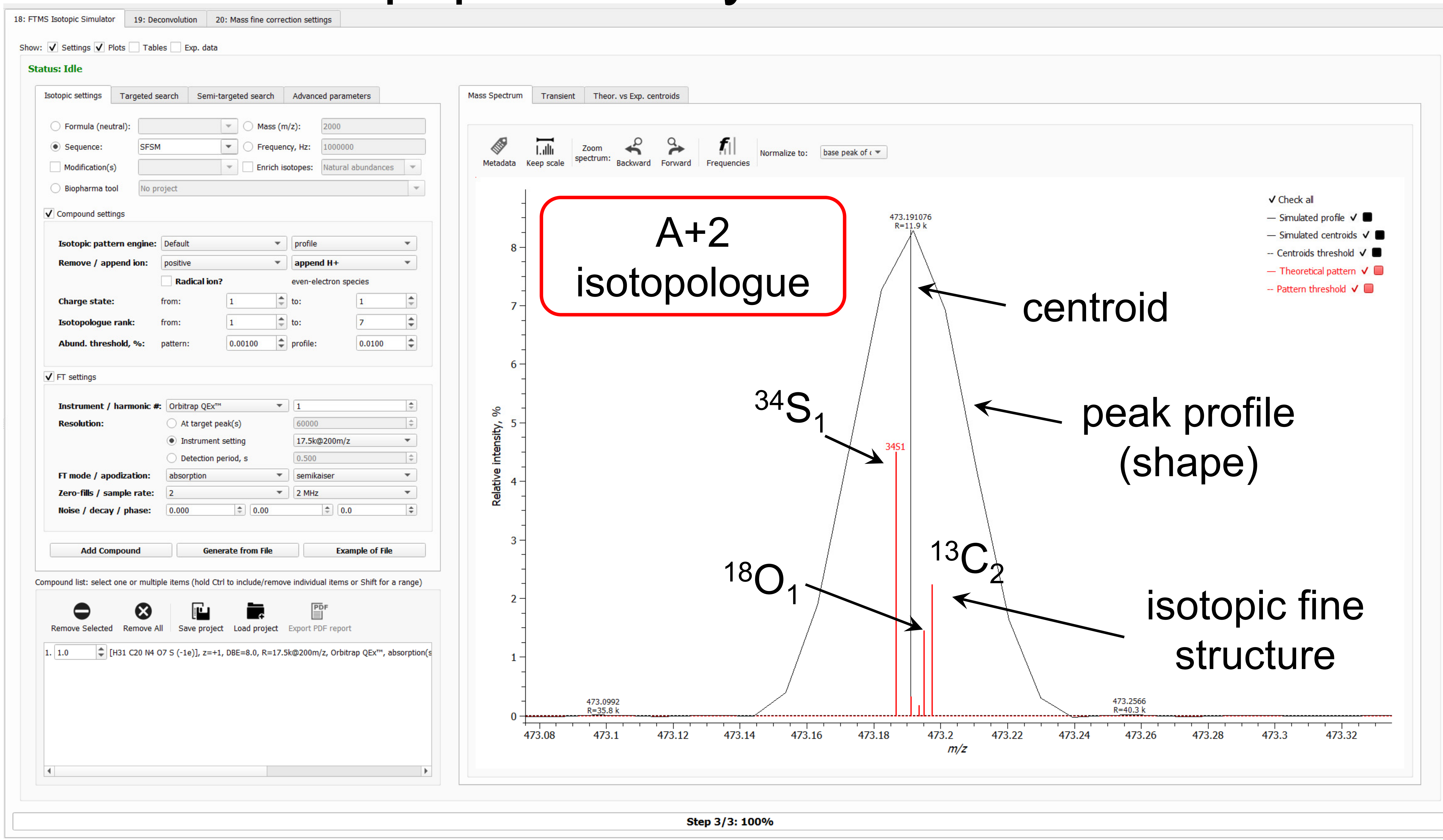
SFSM peptide analysis with FTMS: **frequency**

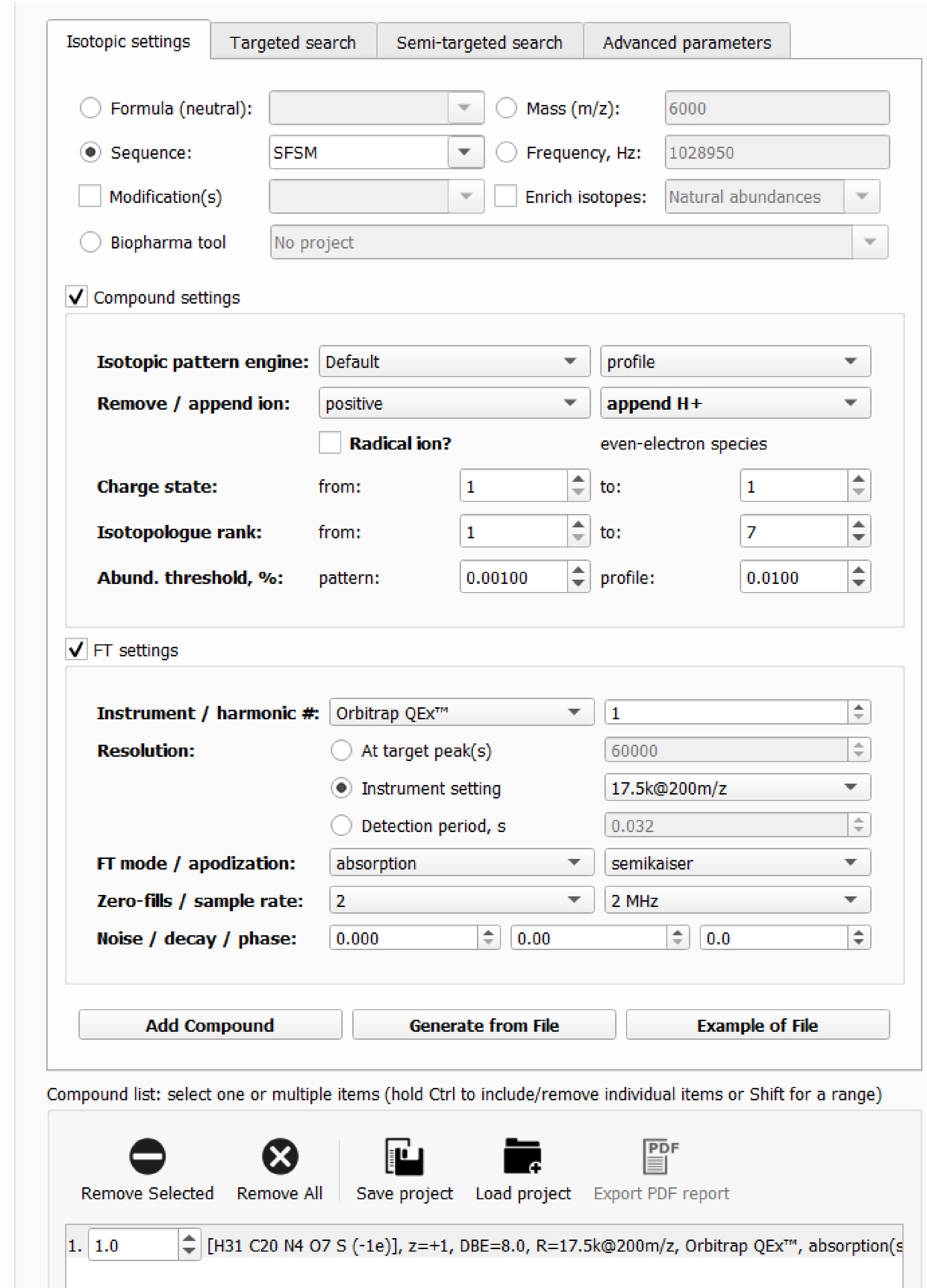


SFSM peptide analysis with FTMS: *m/z*



SFSM peptide analysis with FTMS: *m/z*





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Compound definition:

- elemental composition
- amino acid sequence
- mass (*m/z*) or frequency value

Ion (charged compound) definition:

- Charge carrier: electron, H^+, K^+, Na^+, Cs^+, I^-, $HCOO^-$
- Ionization mode: positive, negative, or a neutral species
- Charge state: from the lowest to the highest
- Isotopologues: how many and which ones

FT processing settings:

- FTMS instrument and model: ICR/MRMS, Orbitraps
- Harmonics order: which harmonic to calculate
- Resolution: at target peak, instrument setting, transient length
- FT mode: absorption or magnitude
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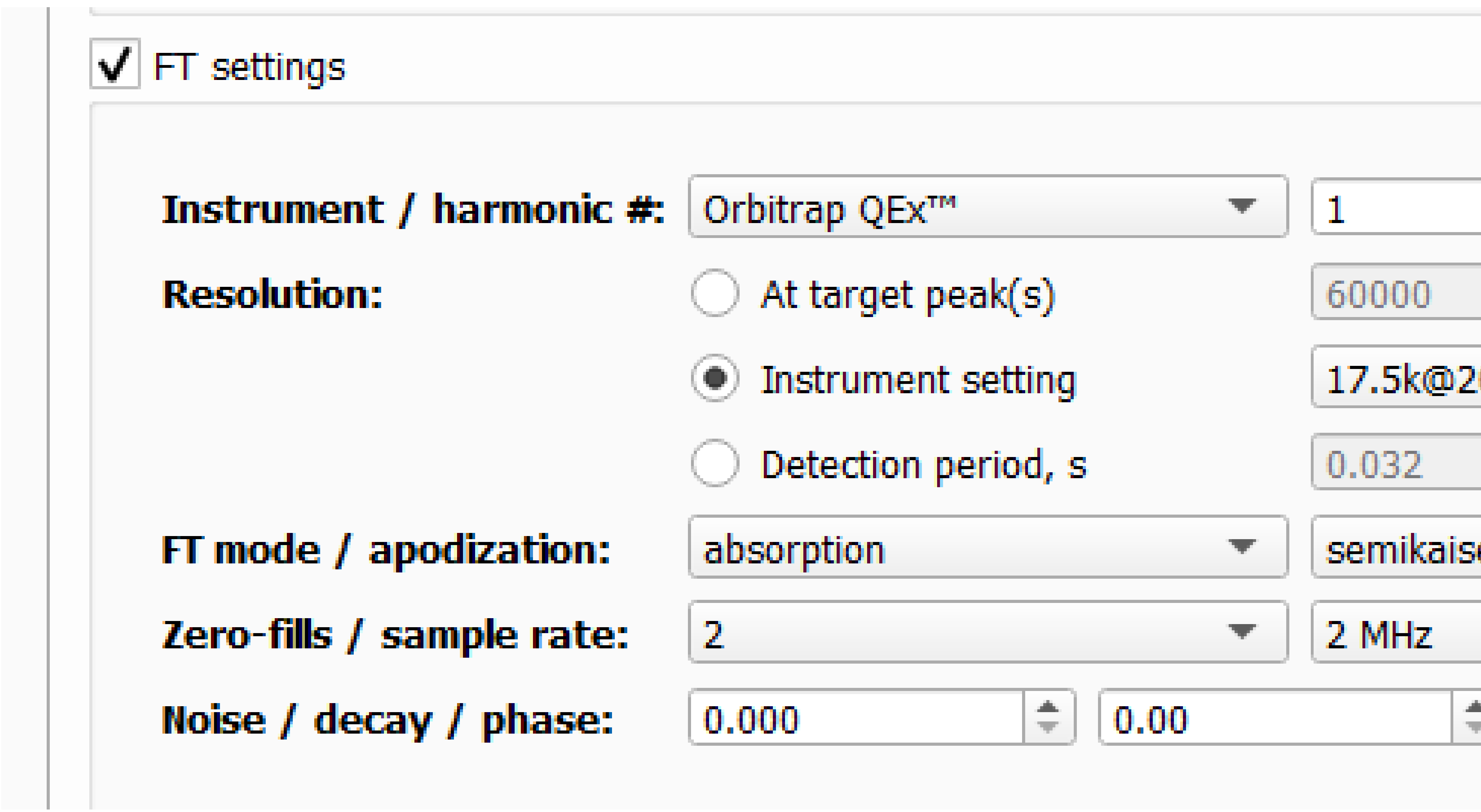
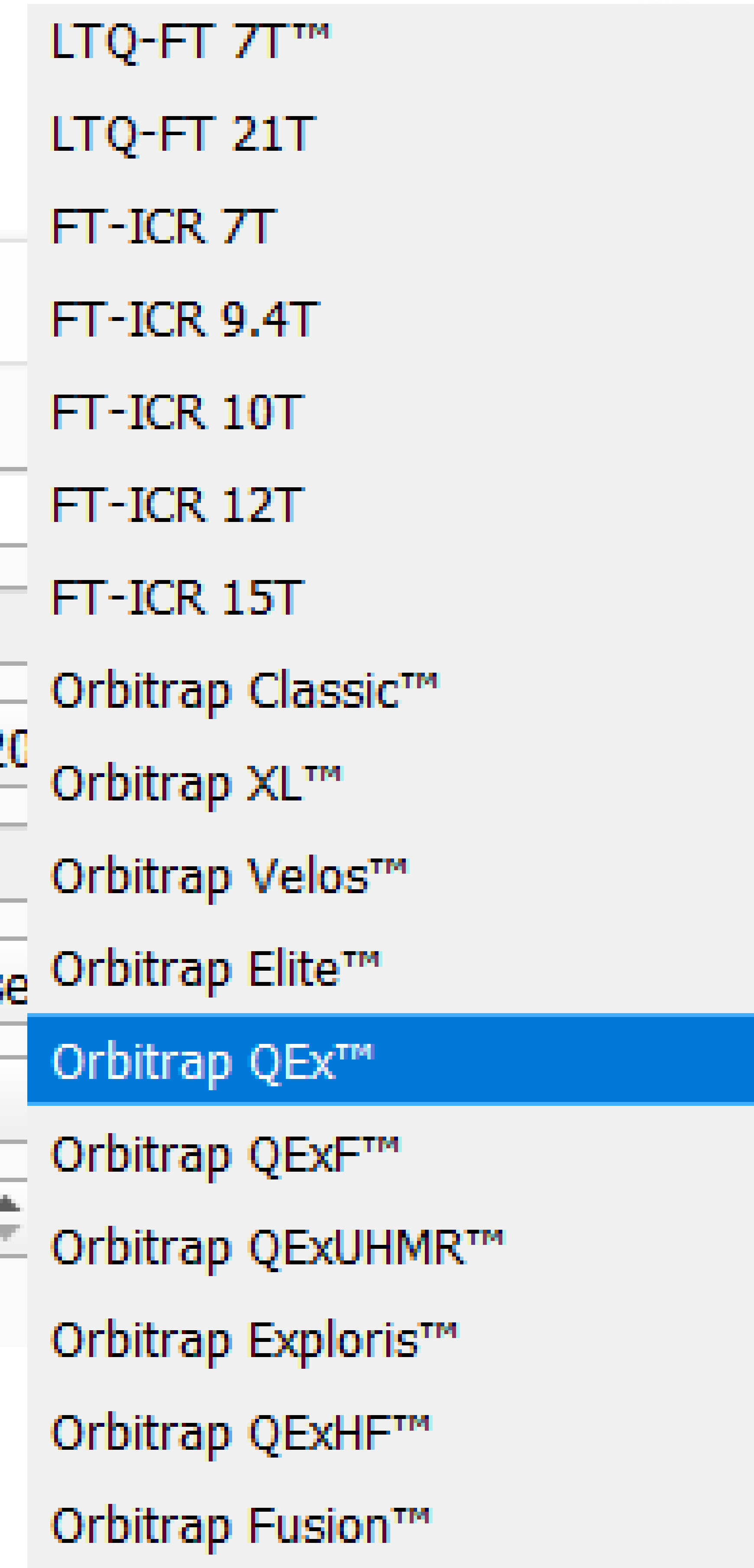
- Number of zero fills: 0, 1, 2, or 3
- Sampling rate (digitization frequency): 1, 2, 4, or 6 MHz, or any
- Noise (added to the transient): noise amplitude
- Decay rate: ion signal decay rate in a transient, $e^{-(\text{decay rate})}$
- Phase: initial phase (angle) of ion detection in a transient

FT Processing Settings: **Frequency**



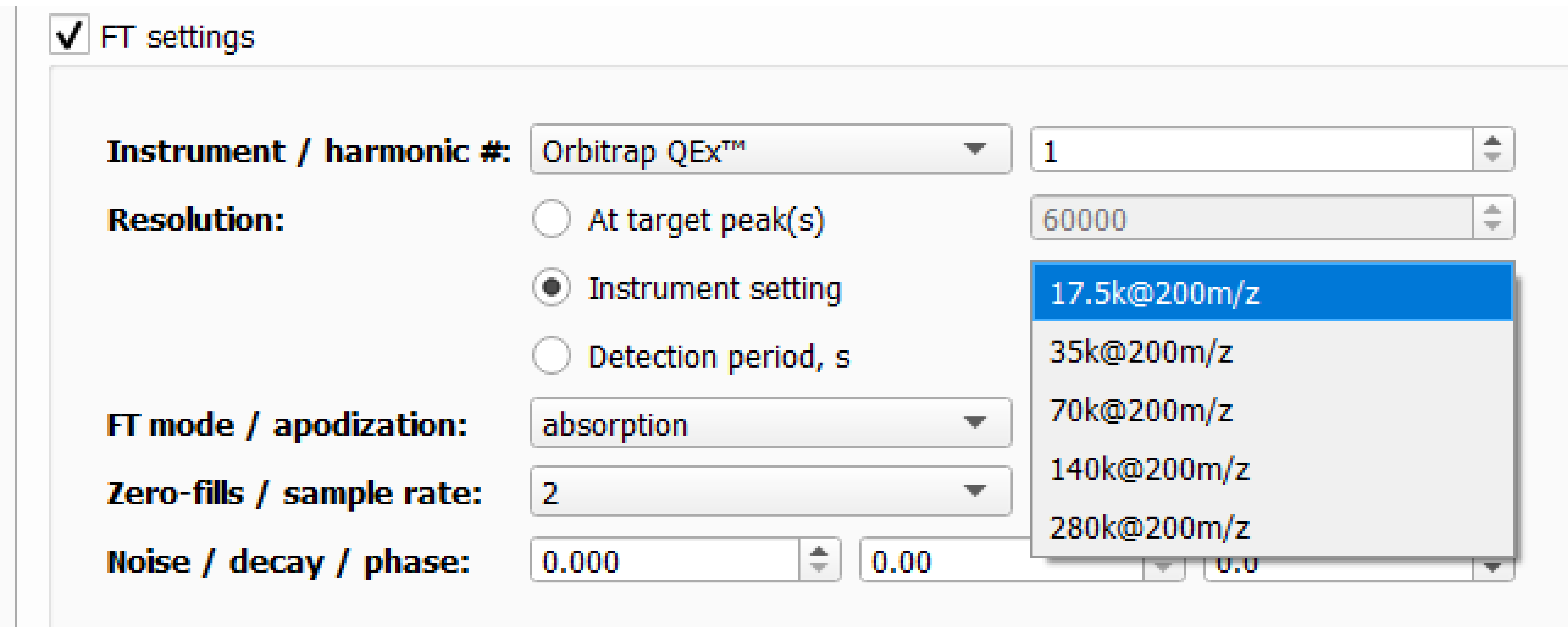


Orbitrap models: https://planetorbitrap.com/

Spectroswiss

FT Processing Settings: **Resolution**

- **Orbitrap** resolution settings are typically estimated at *m/z* 200 (eFT mode)
- The original LTQ Orbitrap models estimate resolution at *m/z* 400 (mFT or eFT)



Spectroswiss

Resolution = *f* (transient period)

Transient length, ms	Resolution @ 200 *m/z* (eFT mass spectra, 5 kV potential)		
	Q Exactive (Plus, Focus, UHMR): D30	Q Exactive HF (GC): D20	Fusion (Lumos, ID-X, Eclipse): D20
16	-	7,500 (only Exploris)	7,500 (only Eclipse)
32	-	15,000	15,000
64	17,500	30,000	30,000
128	35,000	60,000	60,000
256	70,000	120,000	120,000
512	140,000	240,000	240,000
1,024	280,000 (only QEx+)	480,000 (only Exploris)	500,000
2,048	-	-	1000,000 (only 1M)

$$R \approx f \cdot T$$

$$f_{Orbitrap} \propto \frac{1}{\sqrt{m/z}}$$

Spectroswiss

Resolution = *f* (transient period)

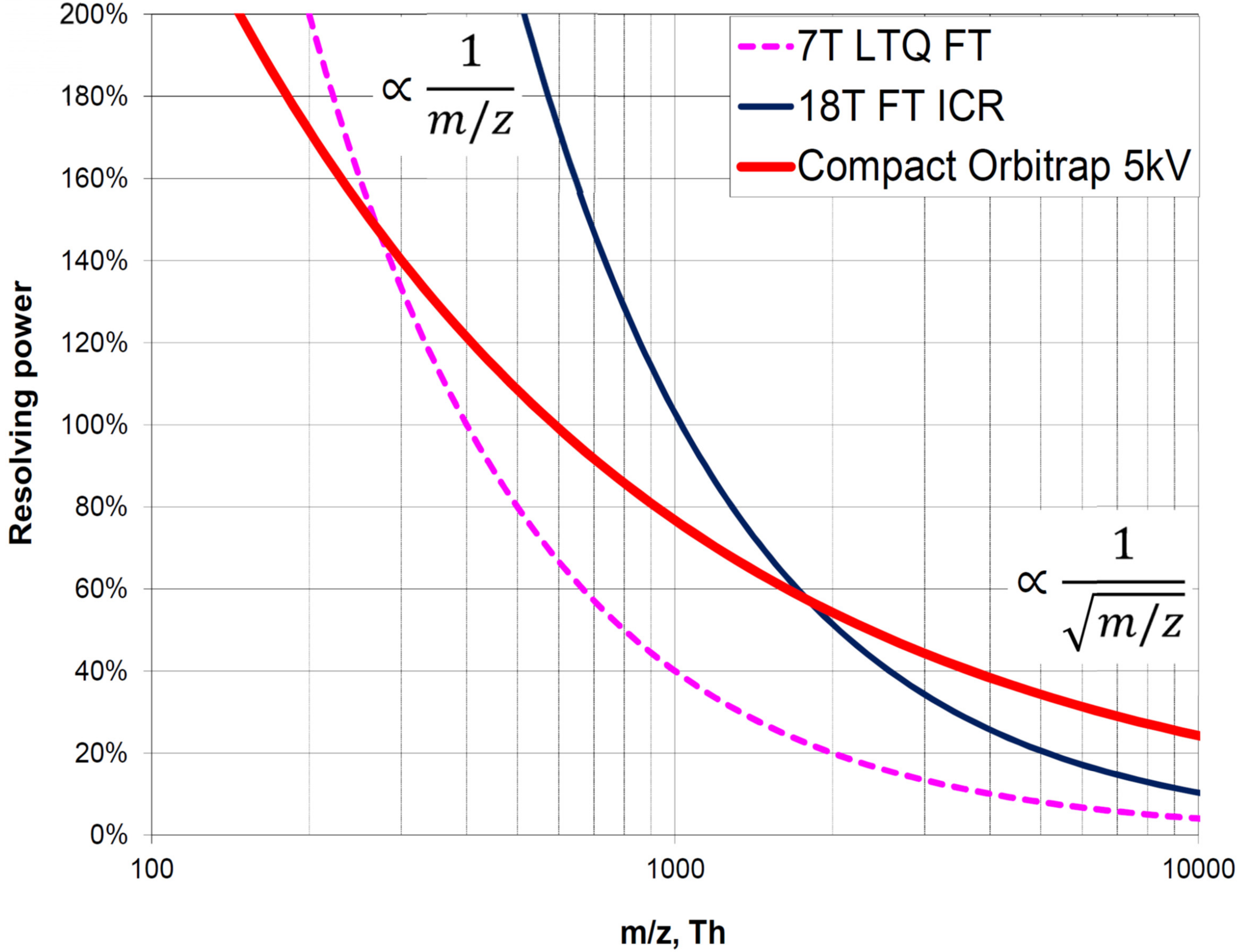
Transient length, ms	Resolution @ 400 *m/z*		
	LTQ Orbitrap XL/Velos (mFT, 3.5 kV): D30	LTQ Orbitrap Elite (eFT, 3.5 kV): D20	Compact, high-field (eFT, 5 kV): D20
48	-	15,000	18,000
96	7,500	30,000	35,500
192	15,000	60,000	71,000
384	30,000	120,000	142,000
768	60,000	240,000	282,000
1536	100,000	480,000	560,000
3072	-	1 M	1100,000

$$R \approx f \cdot T$$

$$f_{Orbitrap} \propto \frac{1}{\sqrt{m/z}}$$

Spectroswiss

Resolution = function of frequency or *m/z*



$$R \propto f \cdot T$$

$$f_{ICR} \propto \frac{1}{m/z}$$

$$f_{Orbitrap} \propto \frac{1}{\sqrt{m/z}}$$

Resolution: ICR vs. Orbitrap

$$R = \frac{(m/z)}{\Delta(m/z)}$$

$$R_{ICR} \approx \frac{(m/z)}{\Delta(m/z)} = \frac{f}{\Delta f}$$

$$R_{Orbitrap} \approx \frac{(m/z)}{\Delta(m/z)} = \frac{1}{2}\frac{f}{\Delta f}$$

$$f_{ICR} = \frac{A}{(m/z)}$$

$$f_{Orbitrap}^2 = \frac{A}{(m/z)}$$

$$(m/z) = \frac{A}{f}$$

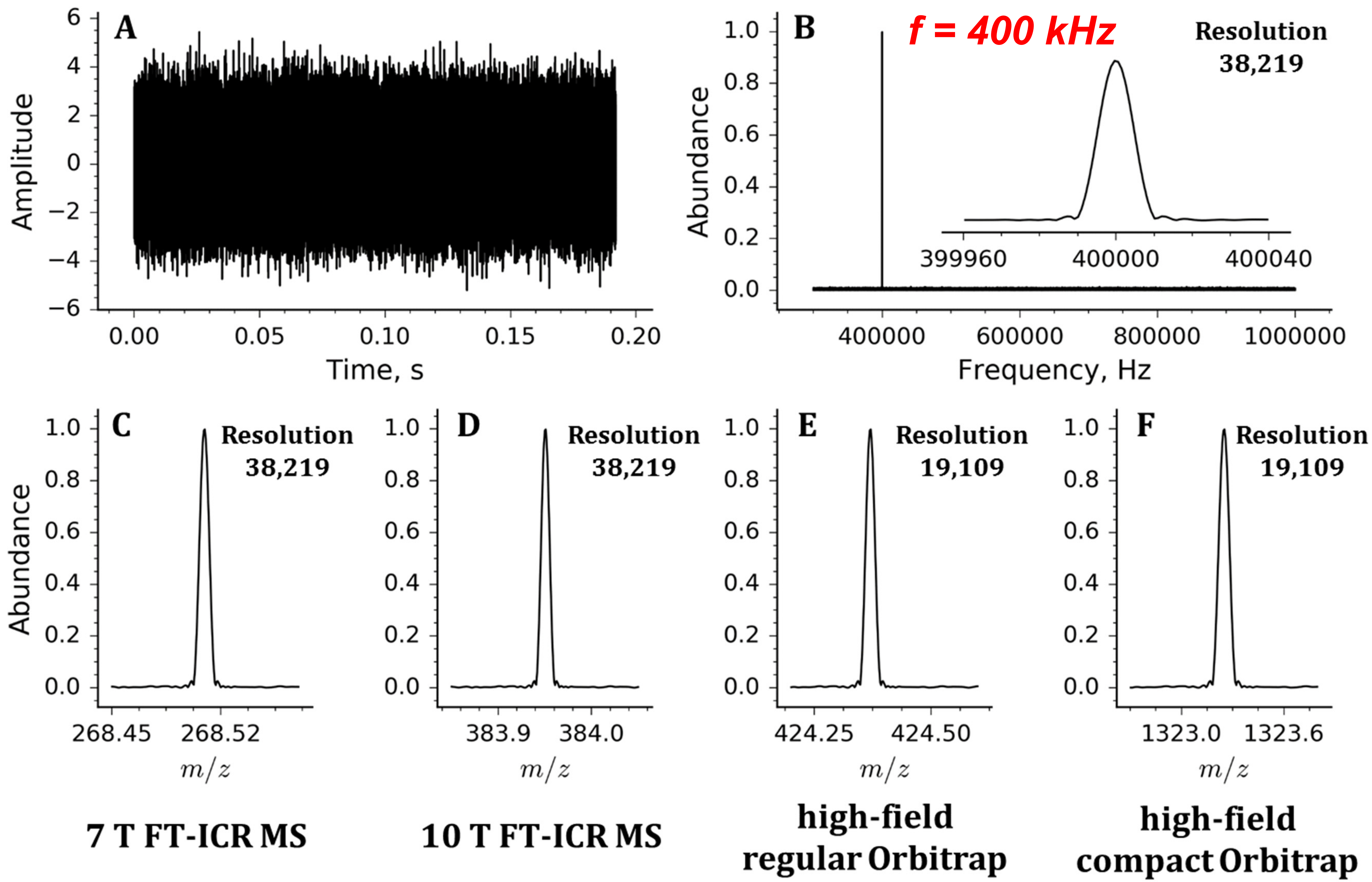
$$(m/z) = \frac{A}{f^2}$$

$$\Delta(m/z) \approx -\frac{A \cdot \Delta f}{f^2} = -(m/z) \cdot \frac{\Delta f}{f}$$

$$\Delta(m/z) \approx -2\frac{A \cdot \Delta f}{f^3} = -2(m/z) \cdot \frac{\Delta f}{f}$$

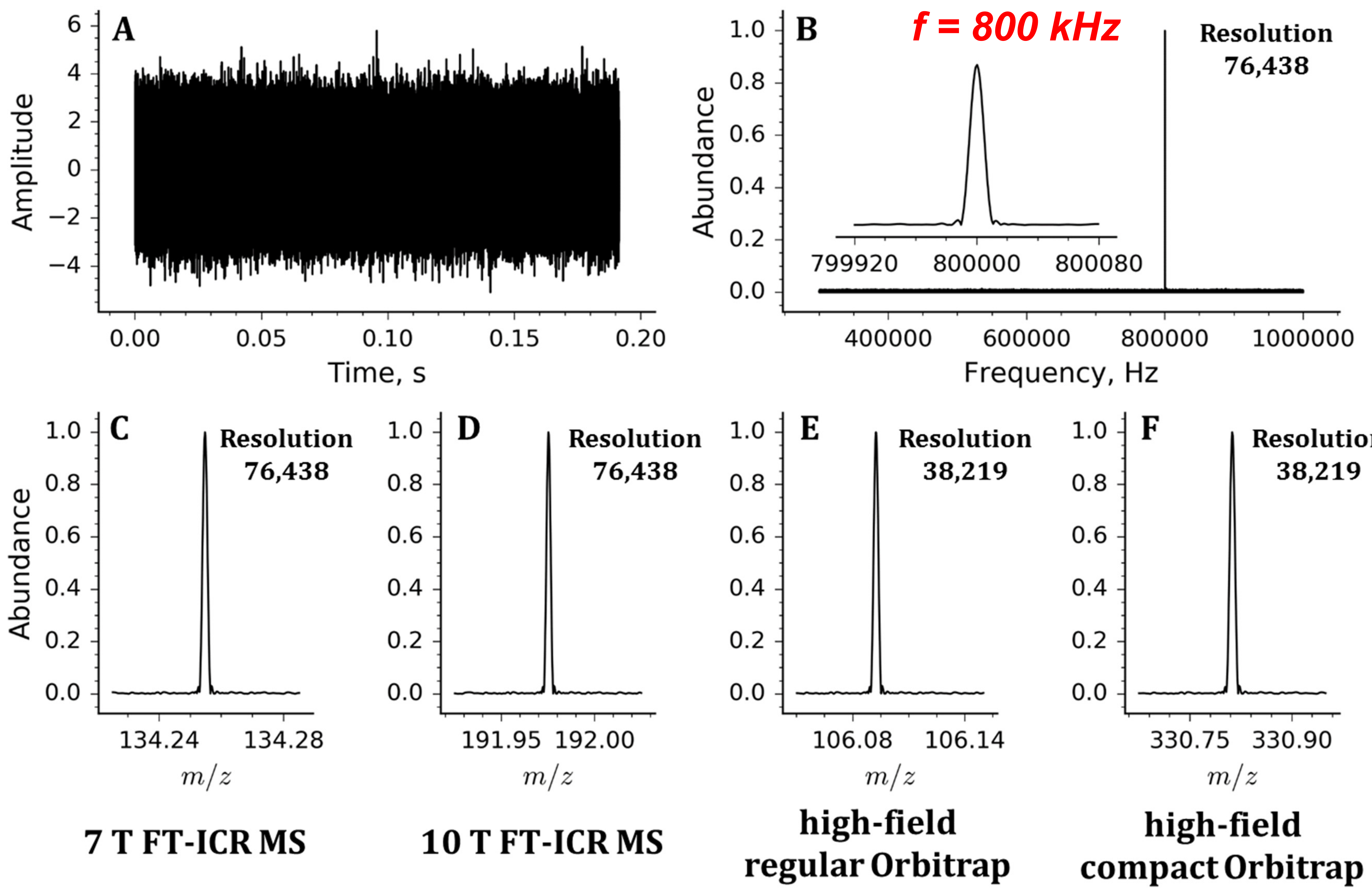
Tsybin *et al. "Advanced FTMS Fundamentals", Chapter 5*

Resolution = Function of *m/z*



Tsybin *et al. “Advanced FTMS Fundamentals”, Chapter 5*

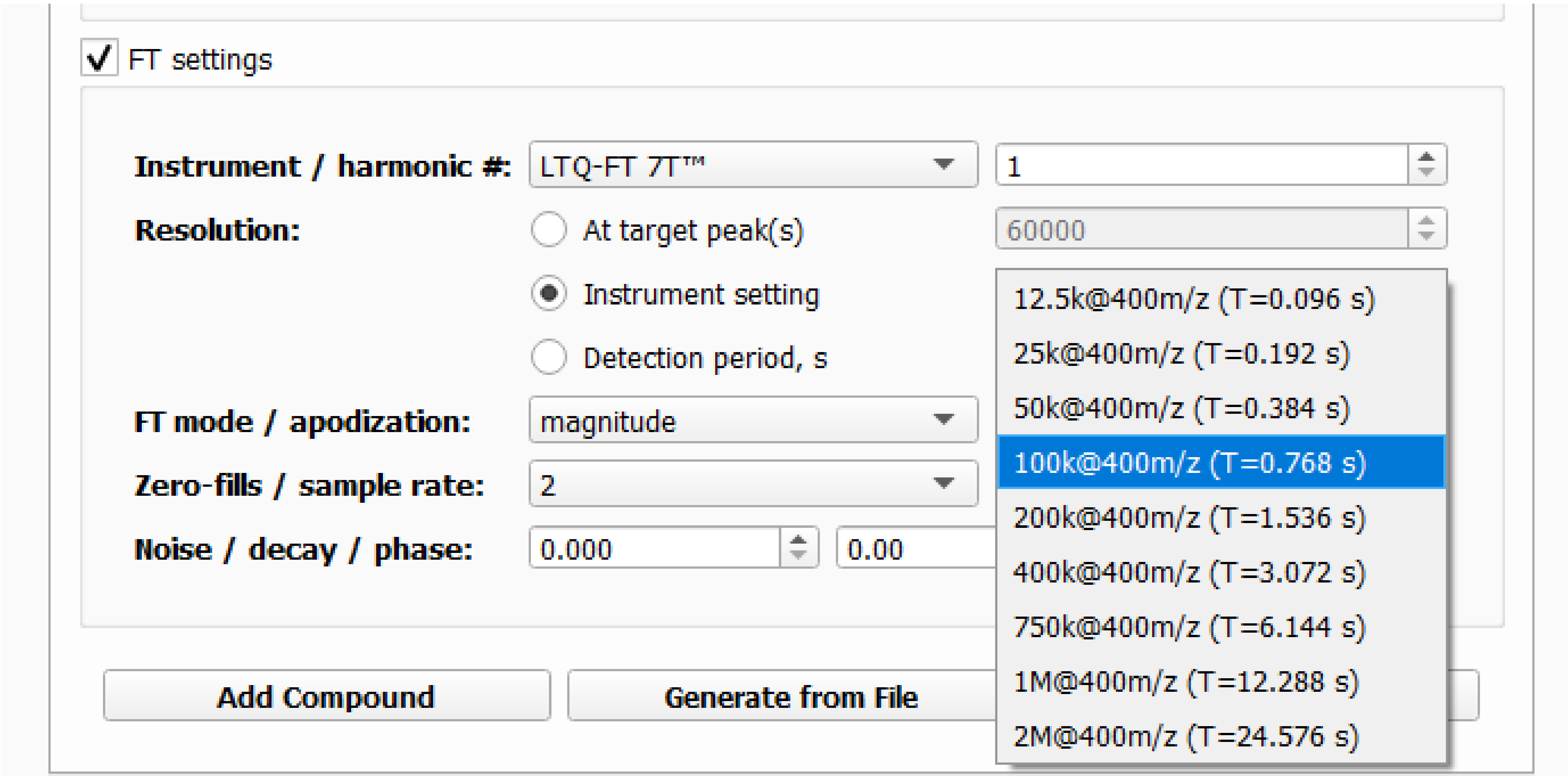
Resolution = Function of *m/z*



Tsybin *et al. “Advanced FTMS Fundamentals”, Chapter 5*

FT Processing Settings: **Resolution**

- **LTQ FT ICR MS** resolution settings are estimated at *m/z* 400 (mFT mode)



FT Processing Settings: **Resolution**

- How to estimate transient length on **Bruker's** ICRs/MRMS?
- Example:

Science of the Total Environment 662 (2019) 852–862

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Petroleomic depth profiling of Staten Island salt marsh soil: 2ω detection FTICR MS offers a new solution for the analysis of environmental contaminants

Mary J. Thomas [a,b], Emma Collinge [b], Matthias Witt [c], Diana Catalina Palacio Lozano [b,d], Christopher H. Vane [e], Vicky Moss-Hayes [e], Mark P. Barrow [b,*]

FT Processing Settings: **Resolution**

- *«Mass spectra were acquired with a 12 T solariX FT-ICR MS. The 4 MW datasets were acquired using magnitude mode, with a detection range of m/z 98 – 3,000. The data were zero-filled once and apodized using a Sine-Bell function prior to applying a fast Fourier transform (FFT). For the apodized data, the measured resolving power at m/z 200 was 650,000.»* **What was the length of the acquired transients?**

$$T_{acq}(s) = \frac{N\ (dataset\ size, MW)}{f_{sampling}, MHz} = \frac{Number\ of\ aquired\ data\ points}{Number\ of\ data\ points\ sampled\ per\ s}$$

$$f_{sampling} = 2 \times f_{highest}$$ **Nyquist**

$$f_{highest} = \frac{1}{2\pi} B \frac{1}{\left({}^{m}/_{q}\right)_{lightest}}$$

$$f_{@12T@98m/z} = 1\,880\,340\ \mathrm{Hz}$$

$$T_{acq} = \frac{4\ \mathrm{MW}}{2 \times 1.88\ \mathrm{MHz}} = \mathbf{1.06\ s}$$

Barrow et al., Science of the Total Environment (2019) 662, 852-862

Spectroswiss

FT Processing Settings: **Resolution**

- *«Mass spectra were acquired with a **7 T** solariX 2xR FT-ICR MS. The **2 MW** datasets were acquired using magnitude mode, with a detection range of **m/z 107** – 3,000. A **2ω** (quadrupolar) ion detection was used. The data were zero-filled once and apodized using a Sine-Bell function prior to applying a fast Fourier transform (FFT). For the apodized data, the measured resolving power at m/z 200 was 300,000.»*

What was the length of the acquired transients?

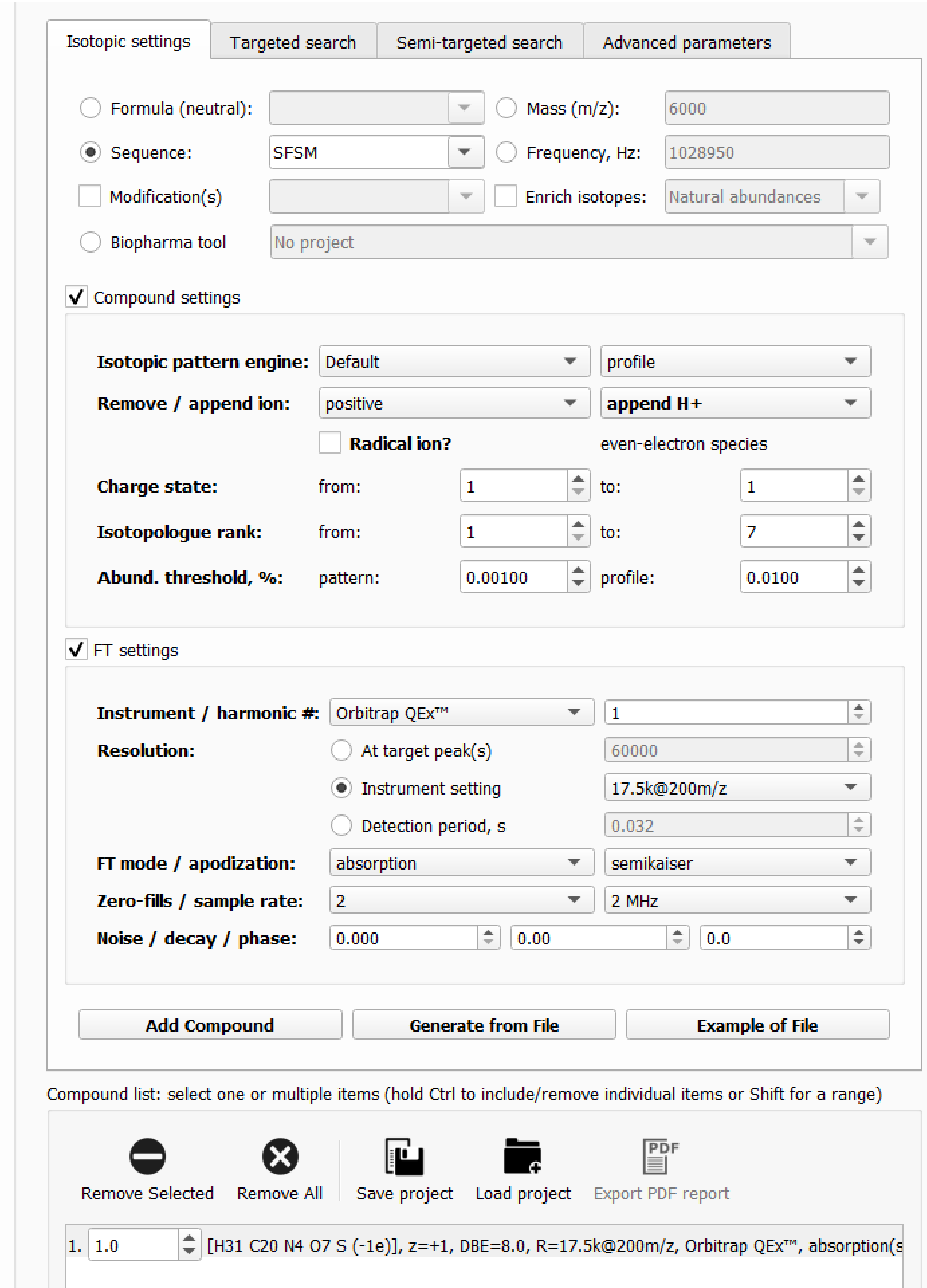
1ω $f_{@7T@107m/z} = 1\,003\,773\ \mathrm{Hz}$

$$T_{acq} = \frac{2\ \mathrm{MW}}{2 \times 1.004\ \mathrm{MHz}} = \mathbf{1\ s}$$

2ω $f_{@7T@107m/z} = 2\,007\,547\ \mathrm{Hz}$

$$T_{acq} = \frac{2\ \mathrm{MW}}{2 \times 2.007\ \mathrm{MHz}} = \mathbf{0.5\ s}$$

Barrow et al., Science of the Total Environment (2019) 662, 852-862



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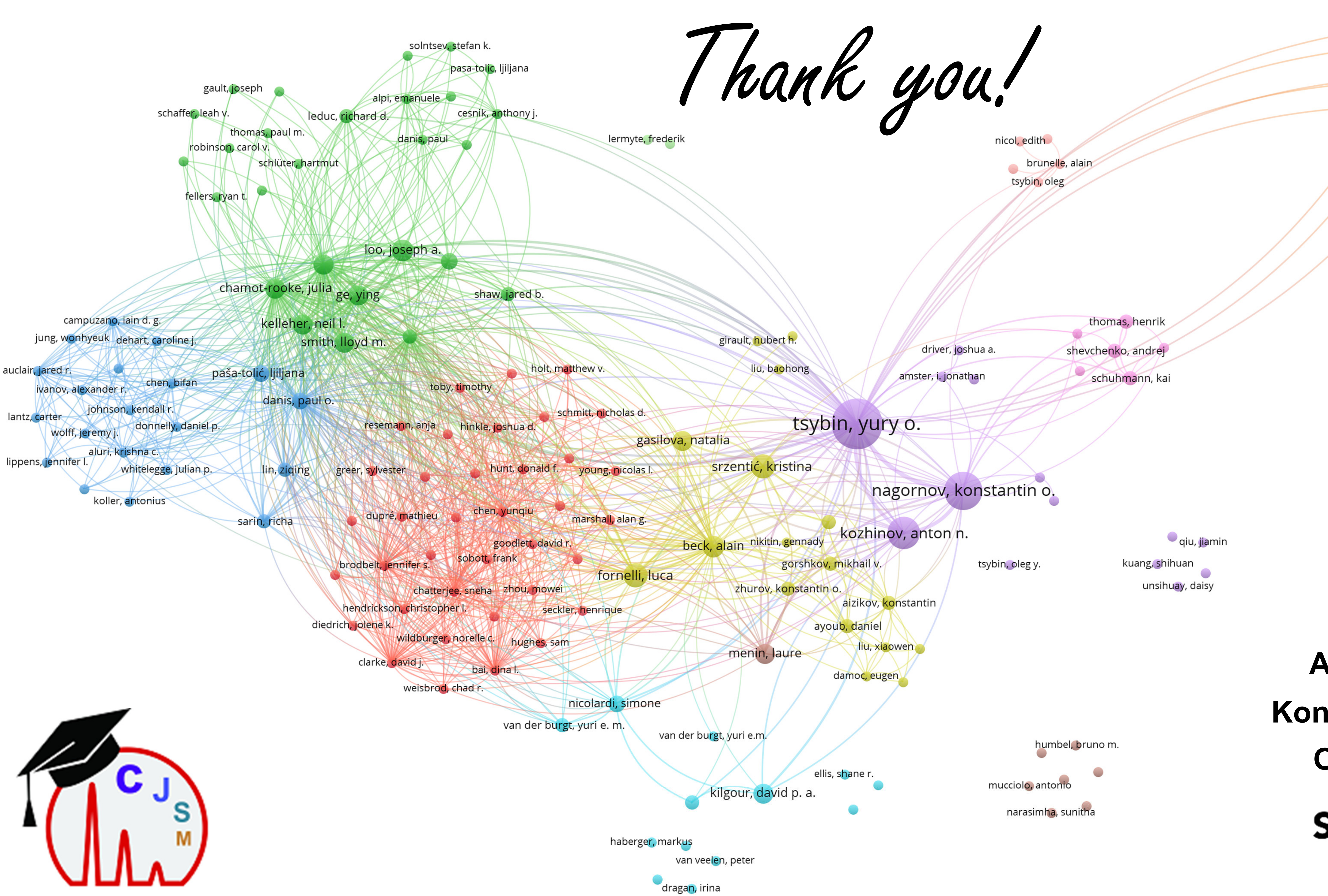
FTMS Fundamentals and Data Processing

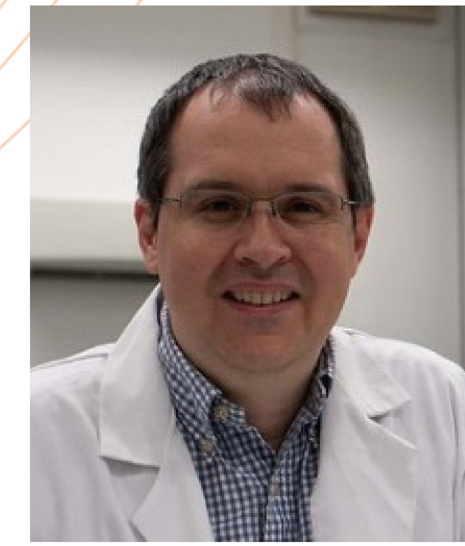
Suggested Reading

- Fourier transform ion cyclotron resonance mass spectrometry: a primer. *Mass Spectrometry Reviews* (1998) 17:1-35
- Fourier Transform Mass Spectrometry. *Molecular & Cellular Proteomics* (2011) 10:M111.009431
- Advanced fundamentals in Fourier transform mass spectrometry. Chapter 5. DOI: 10.1016/B978-0-12-814013-0.00005-3
- Data processing in Fourier transform ion cyclotron resonance mass spectrometry. *Mass Spectrom. Reviews* (2014) 33:333-352
- Fourier transform ion cyclotron resonance mass spectrometry at the true cyclotron frequency. *Mass Spectrom. Reviews* (2021)
- Enhanced Fourier transform for Orbitrap mass spectrometry. *Int. J. Mass Spectrom.* (2014) 369, 15, 16-22
- Performance evaluation of a high-field orbitrap mass analyzer. *J. Amer. Soc. Mass Spectrom.* (2009) 20, 1391-1396
- Dynamics of ions of intact proteins in the Orbitrap mass analyzer. *J. Amer. Soc. Mass Spectrom.* (2009) 20, 1486-1495
- Absorption mode Fourier transform for FTMS: http://www.kilgourlab.com/absorption-mode-for-ft-ms/
- Transient-mediated simulations of FTMS isotopic distributions and mass spectra to guide experiment design and data analysis. *J. Amer. Soc. Mass Spectrom.* (2020) 31, 1927-1942
- Multiplexed MS of individual ions improves measurement of proteoforms and their complexes. DOI: 10.1038/s41592-020-0764-5
- Resource on Orbitrap models design and applications: https://planetorbitrap.com/

Quiz results, software access, questions, & ideas: tsybin@spectroswiss.ch

Thank you!





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CJSM