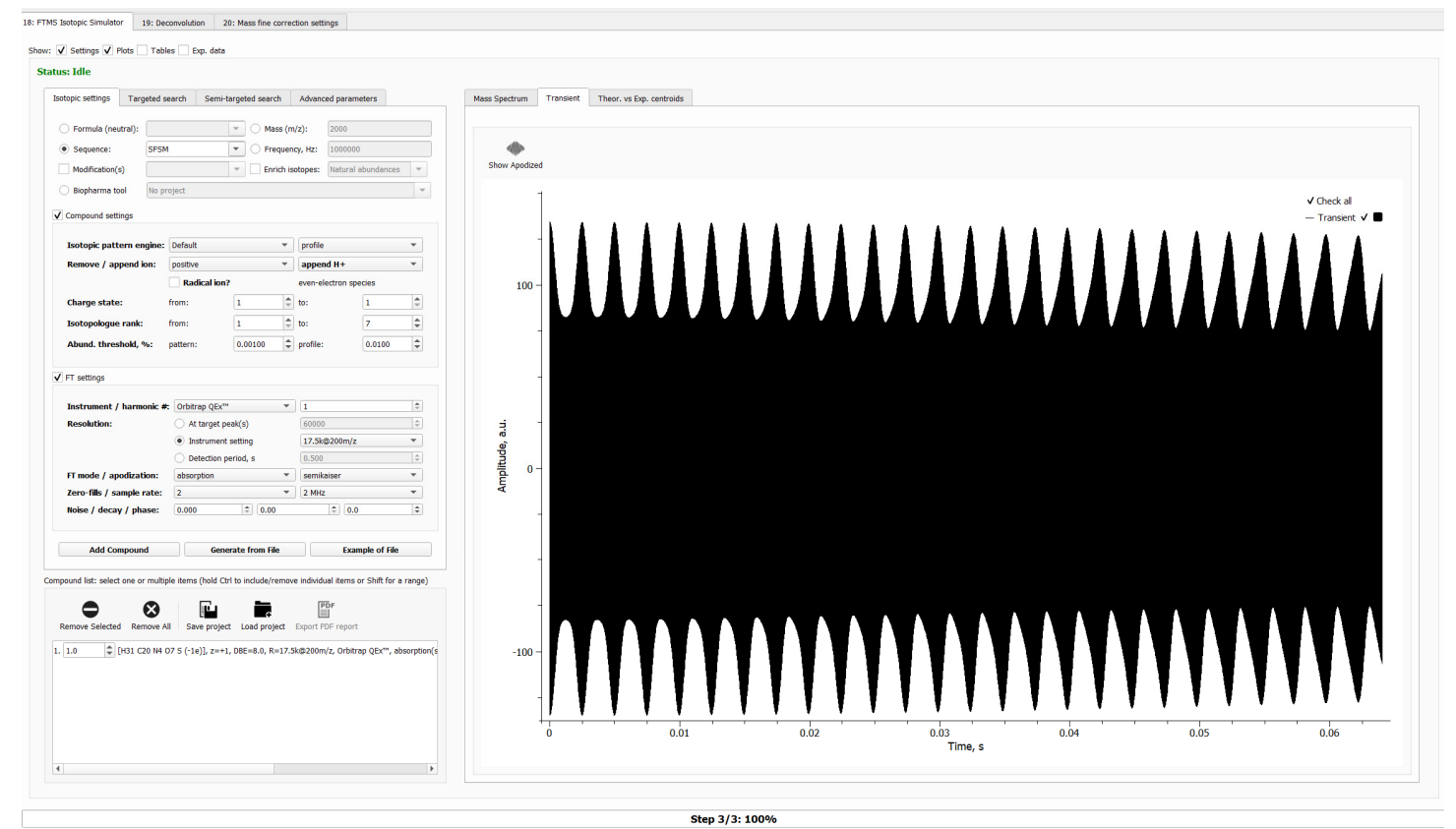
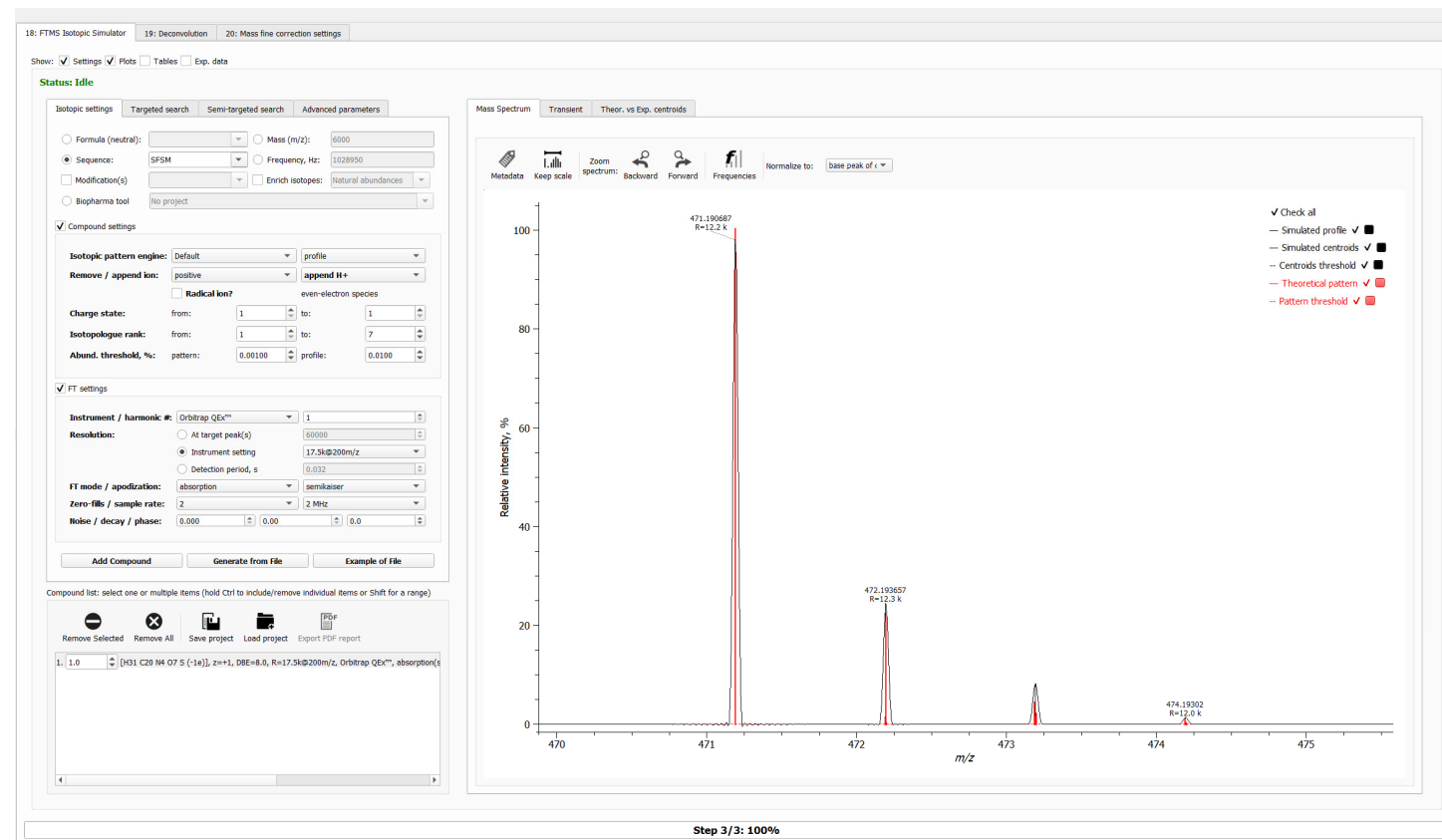


## Application Note #1

# FTMS Simulator: Step-by-Step FTMS Data Generation



# FTMS Isotopic Simulator: SFSM Peptide Analysis

18: FTMS Isotopic Simulator 19: Deconvolution 20: Mass fine correction settings

Show:  Settings  Plots  Tables  Exp. data

Status: Idle

Isotopic settings Targeted search Semi-targeted search Advanced parameters

Formula (neutral):   Mass (m/z): 6000

Sequence: SFSM  Frequency, Hz: 1028950

Modification(s)  Enrich isotopes: Natural abundances

Biopharma tool: No project

Compound settings

Isotopic pattern engine: Default profile

Remove / append ion: positive append H+

Radical ion? even-electron species

Charge state: from: 1 to: 1

Isotopologue rank: from: 1 to: 7

Abund. threshold, %: pattern: 0.00100 profile: 0.0100

FT settings

Instrument / harmonic #: Orbitrap QEx™ 1

Resolution:  At target peak(s) 60000  
 Instrument setting 17.5k@200m/z  
 Detection period, s 0.032

FT mode / apodization: absorption semikaiser

Zero-fills / sample rate: 2 2 MHz

Noise / decay / phase: 0.000 0.00 0.0

Add Compound Generate from File Example of File

Compound list: select one or multiple items (hold Ctrl to include/remove individual items or Shift for a range)

Remove Selected Remove All Save project Load project Export PDF report

1. 1.0 [H31 C20 N4 O7 S (-1e)], z=+1, DBE=8.0, R=17.5k@200m/z, Orbitrap QEx™, absorption(s)

Mass Spectrum Transient Theor. vs Exp. centroids

Metadata Keep scale Zoom spectrum: Backward Forward Frequencies Normalize to: base peak of c

Relative intensity, %

471.190687  
R=12.2 k

472.193657  
R=12.3 k

474.19302  
R=12.0 k

470 471 472 473 474 475  
m/z

✓ Check all  
— Simulated profile ✓   
— Simulated centroids ✓   
— Centroids threshold ✓   
— Theoretical pattern ✓   
— Pattern threshold ✓

Step 3/3: 100%

# SFSM peptide analysis with FTMS: transient

18: FTMS Isotopic Simulator    19: Deconvolution    20: Mass fine correction settings

Show:  Settings  Plots  Tables  Exp. data

Status: Idle

Isotopic settings    Targeted search    Semi-targeted search    Advanced parameters

Formula (neutral):      Mass (m/z): 2000  
 Sequence: SFSM     Frequency, Hz: 1000000  
 Modification(s)      Enrich isotopes: Natural abundances  
 Biopharma tool: No project

Compound settings

Isotopic pattern engine: Default    profile  
Remove / append ion: positive    append H+  
 Radical ion?    even-electron species  
Charge state: from: 1    to: 1  
Isotopologue rank: from: 1    to: 7  
Abund. threshold, %: pattern: 0.00100    profile: 0.0100

FT settings

Instrument / harmonic #: Orbitrap QEx™    1  
Resolution:  At target peak(s) 60000  
 Instrument setting 17.5k@200m/z  
 Detection period, s 0.500  
FT mode / apodization: absorption    semikaizer  
Zero-fills / sample rate: 2    2 MHz  
Noise / decay / phase: 0.000    0.00    0.0

Add Compound    Generate from File    Example of File

Compound list: select one or multiple items (hold Ctrl to include/remove individual items or Shift for a range)

Remove Selected    Remove All    Save project    Load project    Export PDF report

1. 1.0 [H31 C20 N4 O7 S (-1e)], z=+1, DBE=8.0, R=17.5k@200m/z, Orbitrap QEx™, absorption(s)

Mass Spectrum    Transient    Theor. vs Exp. centroids

Show Apodized

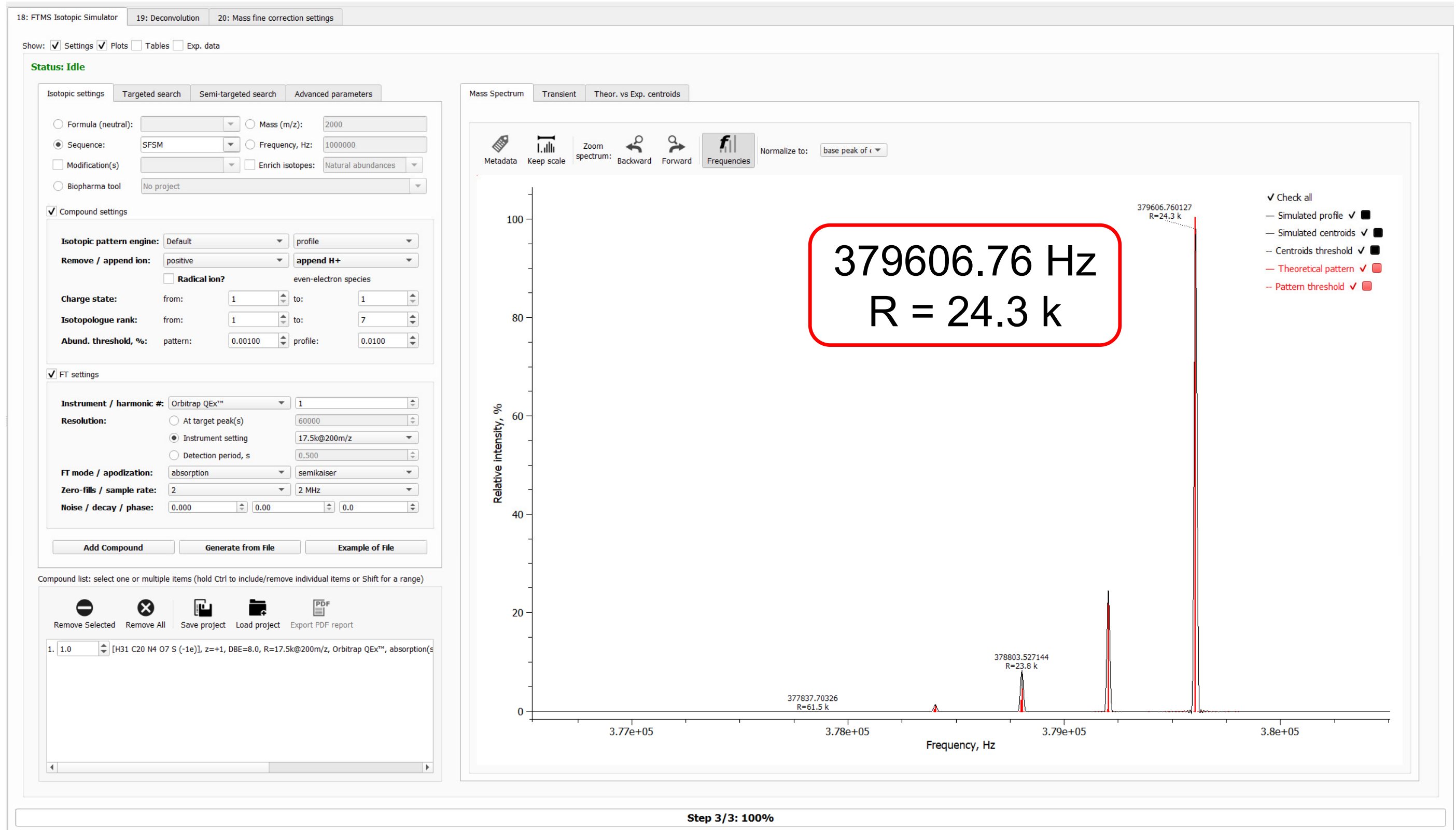
Amplitude, a.u.

Time, s

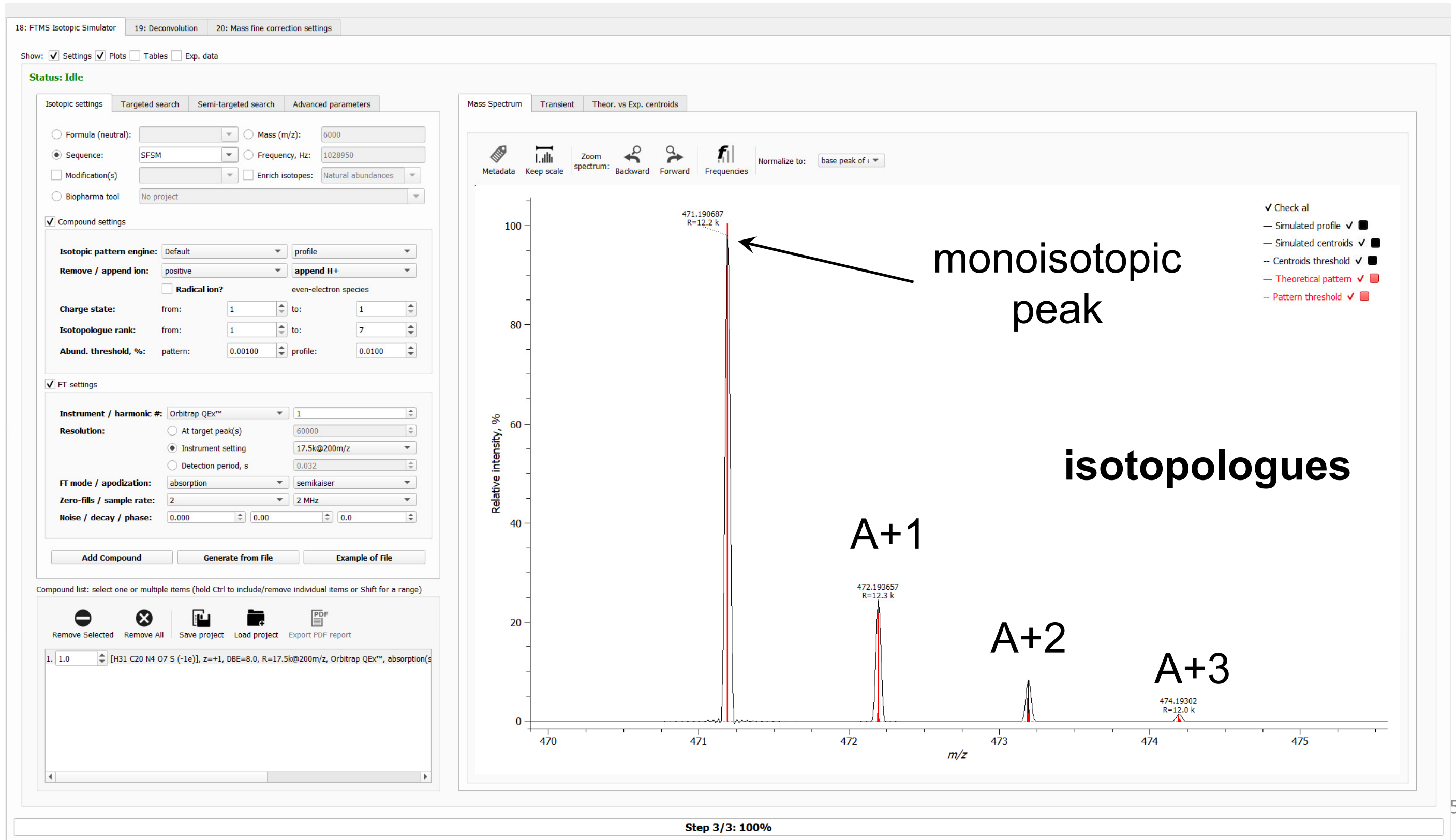
64 ms

Step 3/3: 100%

# SFSM peptide analysis with FTMS: frequency



# SFSM peptide analysis with FTMS: $m/z$



# SFSM peptide analysis with FTMS: $m/z$

18: FTMS Isotopic Simulator    19: Deconvolution    20: Mass fine correction settings

Show:  Settings  Plots  Tables  Exp. data

Status: Idle

Isotopic settings    Targeted search    Semi-targeted search    Advanced parameters

Formula (neutral):     Mass (m/z): 2000

Sequence: SFSM    Frequency, Hz: 1000000

Modification(s):     Enrich isotopes: Natural abundances

Biopharma tool: No project

Compound settings

Isotopic pattern engine: Default    profile

Remove / append ion: positive    append H+

Radical ion?    even-electron species

Charge state: from: 1 to: 1

Isotopologue rank: from: 1 to: 7

Abund. threshold, %: pattern: 0.00100    profile: 0.0100

FT settings

Instrument / harmonic #: Orbitrap QEx™    1

Resolution:  At target peak(s) 60000  
 Instrument setting 17.5k@200m/z  
 Detection period, s 0.500

FT mode / apodization: absorption    semikaiser

Zero-fills / sample rate: 2    2 MHz

Noise / decay / phase: 0.000    0.00    0.0

Add Compound    Generate from File    Example of File

Compound list: select one or multiple items (hold Ctrl to include/remove individual items or Shift for a range)

Remove Selected    Remove All    Save project    Load project    Export PDF report

1. 1.0 [H31 C20 N4 O7 S (-1e)], z=+1, DBE=8.0, R=17.5k@200m/z, Orbitrap QEx™, absorption(s)

---

Mass Spectrum    Transient    Theor. vs Exp. centroids

Metadata    Keep scale    Zoom spectrum: Backward Forward    Frequencies    Normalize to: base peak of  $\epsilon$

Relative intensity, %

**A+2 isotopologue**

centroid

peak profile (shape)

isotopic fine structure

$^{34}\text{S}_1$

$^{18}\text{O}_1$

$^{13}\text{C}_2$

473.191076 R=11.9 k

34S1

473.0992 R=35.8 k

473.2566 R=40.3 k

m/z

Check all

- Simulated profile
- Simulated centroids
- Centroids threshold
- Theoretical pattern
- Pattern threshold

Step 3/3: 100%

Isotopic settings Targeted search Semi-targeted search Advanced parameters

Formula (neutral):   Mass (m/z):

Sequence:   Frequency, Hz:

Modification(s):   Enrich isotopes:

Biopharma tool:

Compound settings

Isotopic pattern engine:

Remove / append ion:

Radical ion? even-electron species

Charge state: from:  to:

Isotopologue rank: from:  to:

Abund. threshold, %: pattern:  profile:

FT settings

Instrument / harmonic #:

Resolution:  At target peak(s)

Instrument setting

Detection period, s

FT mode / apodization:

Zero-fills / sample rate:

Noise / decay / phase:

Compound list: select one or multiple items (hold Ctrl to include/remove individual items or Shift for a range)

1. 1.0 [H31 C20 N4 O7 S (-1e)], z=+1, DBE=8.0, R=17.5k@200m/z, Orbitrap QEx™, absorption(s)

## 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
- Apodization window: none, full (Kaiser), half (semi Kaiser)
- 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

# Compound Definition

Modification(s) / PTM(s)

Name:

Formula:

---

Standard  Glycans

Formula (custom):  0

Formula (custom):  0

Value (custom):  0

Dehydration, -18.01056	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Pyro-glu(Q), -17.02655	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Deoxidation, -15.99491	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
HydrogenLoss, -1.00783	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Amidation, -0.98402	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Deamidation, 0.98402	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Methylation, 14.01565	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Oxidation, 15.99491	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Acetonitrile, 41.02655	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Acetylation, 42.01056	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Carbidomethyl, 57.02146	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Carboxymethyl, 58.00548	0 <input type="button" value="▲"/> <input type="button" value="▼"/>
Isopropanol, 60.05751	0 <input type="button" value="▲"/> <input type="button" value="▼"/>

Isotopic settings  Targeted search  Semi-targeted search  Advanced parameters

Formula (neutral):

Sequence:

Modification(s)

Biopharma tool

Mass (m/z):

Frequency, Hz:

Enrich isotopes:

Isotopic abundances relative to the lightest:

Normalize to number of atoms

1H:	1 <input type="button" value="▲"/> <input type="button" value="▼"/>	2H:	0.000115 <input type="button" value="▲"/> <input type="button" value="▼"/>				
12C:	1 <input type="button" value="▲"/> <input type="button" value="▼"/>	13C:	0.010816 <input type="button" value="▲"/> <input type="button" value="▼"/>				
14N:	1 <input type="button" value="▲"/> <input type="button" value="▼"/>	15N:	0.003653 <input type="button" value="▲"/> <input type="button" value="▼"/>				
16O:	1 <input type="button" value="▲"/> <input type="button" value="▼"/>	17O:	0.000381 <input type="button" value="▲"/> <input type="button" value="▼"/>	18O:	0.002055 <input type="button" value="▲"/> <input type="button" value="▼"/>		
32S:	1 <input type="button" value="▲"/> <input type="button" value="▼"/>	33S:	0.007896 <input type="button" value="▲"/> <input type="button" value="▼"/>	34S:	0.044742 <input type="button" value="▲"/> <input type="button" value="▼"/>	36S:	0.000105 <input type="button" value="▲"/> <input type="button" value="▼"/>



# Compound Definition

Isotopic settings   Targeted search   Semi-targeted search   Advanced parameters

Formula (neutral):

Sequence:

Modification(s)

Biopharma tool

Biopharma FT simulations

Intact   Top-down

Light chain #2: H1598 C1032 N277 O335 S6, 23423.48472 Da

```
N D I Q M T Q S P S S L S A S V G D R V T 20
21 I T C R A S Q D V N T A V A W Y Q Q K P 40
41 G K A P K L L I Y S A S F L Y S G V P S 60
61 R F S G S R S G T D F T L T I S S L Q P 80
81 E D F A T Y Y C Q Q H Y T T P P T F G Q 100
101 G T K V E I K R T V A A P S V F I F P P 120
121 S D E Q L K S G T A S V V C L L N N F Y 140
141 P R E A K V Q W K V D N A L Q S G N S Q 160
161 E S V T E Q D S K D S T Y S L S S T L T 180
181 L S K A D Y E K H K V Y A C E V T H Q G 200
201 L S S P V T K S F N R G E C
```

Light chain #1: H1598 C1032 N277 O335 S6, 23423.48472 Da

```
N D I Q M T Q S P S S L S A S V G D R V T 20
21 I T C R A S Q D V N T A V A W Y Q Q K P 40
41 G K A P K L L I Y S A S F L Y S G V P S 60
61 R F S G S R S G T D F T L T I S S L Q P 80
81 E D F A T Y Y C Q Q H Y T T P P T F G Q 100
101 G T K V E I K R T V A A P S V F I F P P 120
121 S D E Q L K S G T A S V V C L L N N F Y 140
141 P R E A K V Q W K V D N A L Q S G N S Q 160
161 E S V T E Q D S K D S T Y S L S S T L T 180
181 L S K A D Y E K H K V Y A C E V T H Q G 200
201 L S S P V T K S F N R G E C
```

mAb type:

Enzyme type:

Compound info: IgG1, Intact

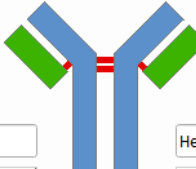
ct: H9972 C6460 N1724 O2014 S44, 145421.5021 Da

Heavy chain #2: H3388 C2198 N585 O672 S16, 49242.44526 Da

```
N E V Q L V E S G G G L V Q P G G S L R L 20
21 S C A A S G F N I K D T Y I H W V R Q A 40
41 P G K G L E W V A R I Y P T N G Y T R Y 60
61 A D S V K G R F T I S A D T S K N T A Y 80
81 L Q M N S L R A E D T A V Y Y C S R W G 100
101 G D G F Y A M D Y W G Q G T L V T V S S 120
121 A S T K G P S V F P L A P S S K S T S G 140
141 G T A A L G C L V K D Y F P E P V T V S 160
161 W N S G A L T S G V H T F P A V L Q S S 180
181 G L Y S L S S V V T V P S S S L G T Q T 200
201 Y I C N V N H K P S N T K V D K K V E P 220
221 K S C D K T H T C P P C P A P E L L G G 240
241 P S V F L F P P K P K D T L M I S R T P 260
261 E V T C V V V D V S H E D P E V K F N W 280
281 Y V D G V E V H N A K T K P R E E Q Y N 300
301 S T Y R V V S V L T V L H Q D W L N G K 320
321 E Y K C K V S N K A L P A P I E K T I S 340
341 K A K G Q P R E P Q V Y T L P P S R E E 360
361 M T K N Q V S L T C L V K G F Y P S D I 380
381 A V E W E S N G Q P E N N Y K T T P P V 400
401 L D S D G S F F L Y S K L T V D K S R W 420
421 Q Q G N V F S C S V M H E A L H N H Y T 440
```

Heavy chain #1: H3388 C2198 N585 O672 S16, 49242.44526 Da

```
N E V Q L V E S G G G L V Q P G G S L R L 20
21 S C A A S G F N I K D T Y I H W V R Q A 40
41 P G K G L E W V A R I Y P T N G Y T R Y 60
61 A D S V K G R F T I S A D T S K N T A Y 80
81 L Q M N S L R A E D T A V Y Y C S R W G 100
101 G D G F Y A M D Y W G Q G T L V T V S S 120
121 A S T K G P S V F P L A P S S K S T S G 140
141 G T A A L G C L V K D Y F P E P V T V S 160
161 W N S G A L T S G V H T F P A V L Q S S 180
181 G L Y S L S S V V T V P S S S L G T Q T 200
201 Y I C N V N H K P S N T K V D K K V E P 220
221 K S C D K T H T C P P C P A P E L L G G 240
241 P S V F L F P P K P K D T L M I S R T P 260
261 E V T C V V V D V S H E D P E V K F N W 280
281 Y V D G V E V H N A K T K P R E E Q Y N 300
301 S T Y R V V S V L T V L H Q D W L N G K 320
321 E Y K C K V S N K A L P A P I E K T I S 340
341 K A K G Q P R E P Q V Y T L P P S R E E 360
361 M T K N Q V S L T C L V K G F Y P S D I 380
381 A V E W E S N G Q P E N N Y K T T P P V 400
401 L D S D G S F F L Y S K L T V D K S R W 420
421 Q Q G N V F S C S V M H E A L H N H Y T 440
```



Compound list: select one or multiple items (hold Ctrl to include/remove individual items or Shift for a range)

1.	1.0	Intact: H9972 C6460 N1724 O2014 S44, 145421.5021 Da
2.	5.0	Intact, G0/G0F: H10146 C6566 N1732 O2088 S44, 148166.027 Da
3.	30.0	Intact, 2xG0F: H10156 C6572 N1732 O2092 S44, 148312.168 Da
4.	55.0	Intact, G0F/G1F: H10166 C6578 N1732 O2097 S44, 148474.309 Da
5.	48.0	Intact, 2xG1F: H10176 C6584 N1732 O2102 S44, 148636.449 Da
6.	11.0	Intact, G1F/G2F: H10186 C6590 N1732 O2107 S44, 148798.590 Da

# Compound Settings

- Set realistic abundance thresholds for the isotopic pattern/profile calculations
- Lower threshold provide higher accuracy simulations, but are computation-heavy

Compound settings

**Isotopic pattern engine:**

Default

profile

**Remove / append ion:**

negative

pattern only

**Radical ion?**

even-electron species

**Charge state:**

from:

1

to:

1

**Isotopologue rank:**

from:

1

to:

7

**Abund. threshold, %:**

pattern:

0.00100

profile:

0.0100

# Compound Settings

- Engine: Speed vs. Accuracy; the more accurate, but slow – default mode
- Use «Turbo (protein mode)» when simulating compounds heavier than 30 kDa

Compound settings

**Isotopic pattern engine:**

Default

Turbo (protein mode)

profile

**Remove / append ion:**

negative

remove H+

**Radical ion?**

even-electron species

**Charge state:**

from:

1

to:

1

**Parameters:**

N isotopes:

1000

# FT Processing Settings: Frequency

FT settings

**Instrument / harmonic #:** Orbitrap QEx™ 1

**Resolution:**

At target peak(s) 60000

Instrument setting 17.5k@20

Detection period, s 0.032

**FT mode / apodization:** absorption semikaise

**Zero-fills / sample rate:** 2 2 MHz

**Noise / decay / phase:** 0.000 0.00

- LTQ-FT 7T™
- LTQ-FT 21T
- FT-ICR 7T
- FT-ICR 9.4T
- FT-ICR 10T
- FT-ICR 12T
- FT-ICR 15T
- Orbitrap Classic™
- Orbitrap XL™
- Orbitrap Velos™
- Orbitrap Elite™
- Orbitrap QEx™**
- Orbitrap QExF™
- Orbitrap QExUHMR™
- Orbitrap Exploris™
- Orbitrap QExHF™
- Orbitrap Fusion™

Orbitrap models: <https://planetorbitrap.com/>

# 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)

FT settings

**Instrument / harmonic #:**

Orbitrap QEx™

1

**Resolution:**

At target peak(s)

60000

Instrument setting

Detection period, s

17.5k@200m/z

35k@200m/z

70k@200m/z

140k@200m/z

280k@200m/z

**FT mode / apodization:**

absorption

**Zero-fills / sample rate:**

2

**Noise / decay / phase:**

0.000

0.00

0.0

# FT Processing Settings: Resolution

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

FT settings

**Instrument / harmonic #:** LTQ-FT 7T™ 1

**Resolution:**

At target peak(s) 60000

Instrument setting

Detection period, s

**FT mode / apodization:** magnitude

**Zero-fills / sample rate:** 2

**Noise / decay / phase:** 0.000 0.00

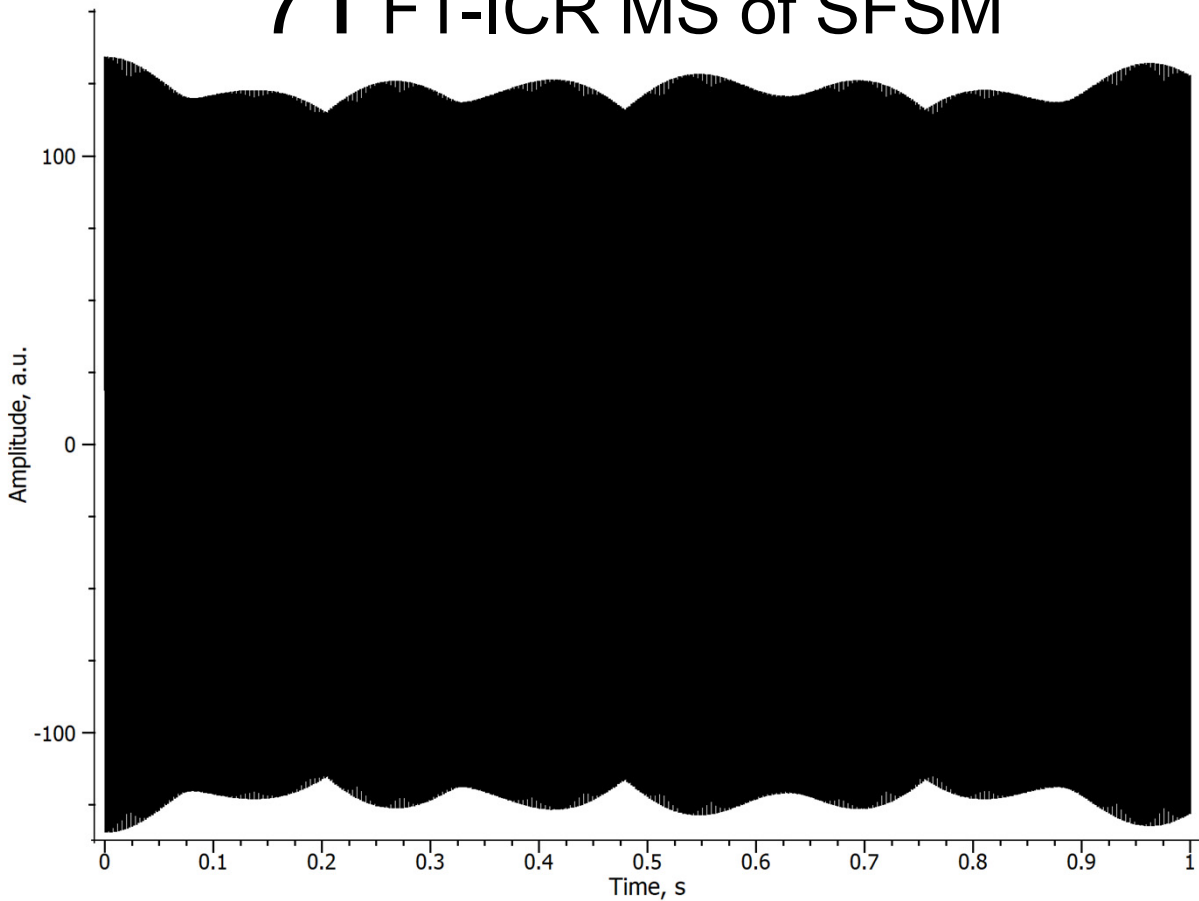
**Resolution List:**

- 12.5k@400m/z (T=0.096 s)
- 25k@400m/z (T=0.192 s)
- 50k@400m/z (T=0.384 s)
- 100k@400m/z (T=0.768 s)**
- 200k@400m/z (T=1.536 s)
- 400k@400m/z (T=3.072 s)
- 750k@400m/z (T=6.144 s)
- 1M@400m/z (T=12.288 s)
- 2M@400m/z (T=24.576 s)


**Add Compound** **Generate from File**

# FT Processing Settings: Decay

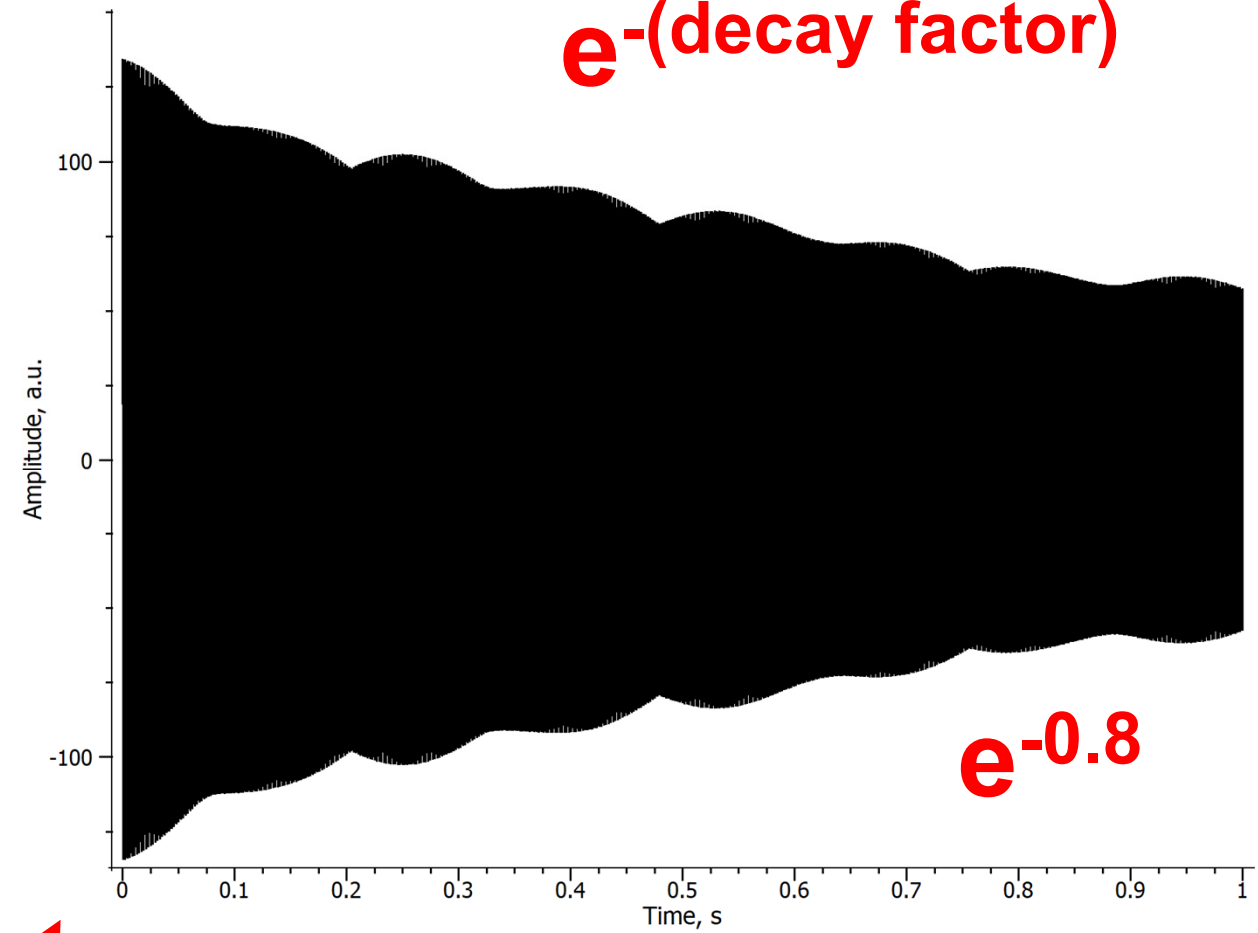
7 T FT-ICR MS of SF5M



space charge  
de-phasing



$e^{-(\text{decay factor})}$

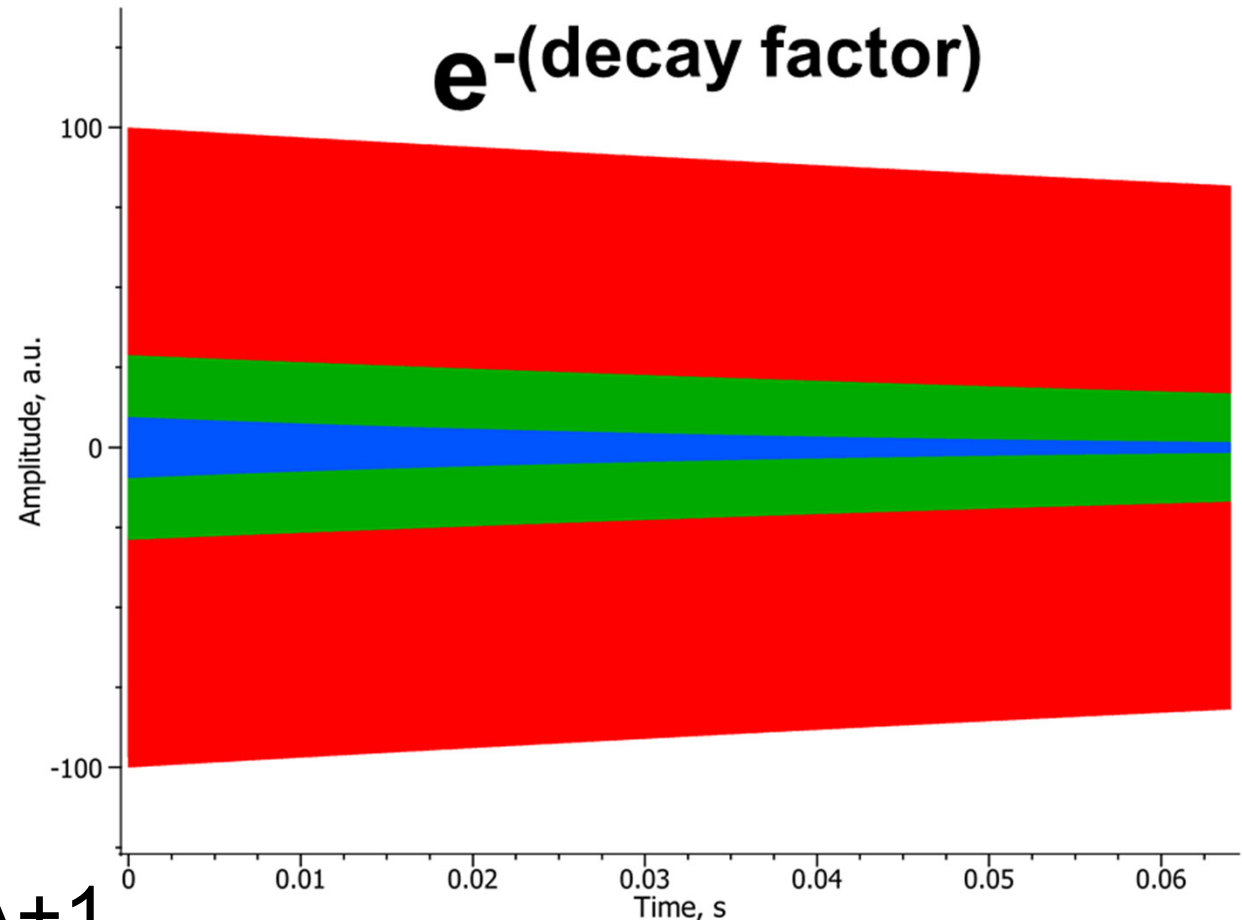
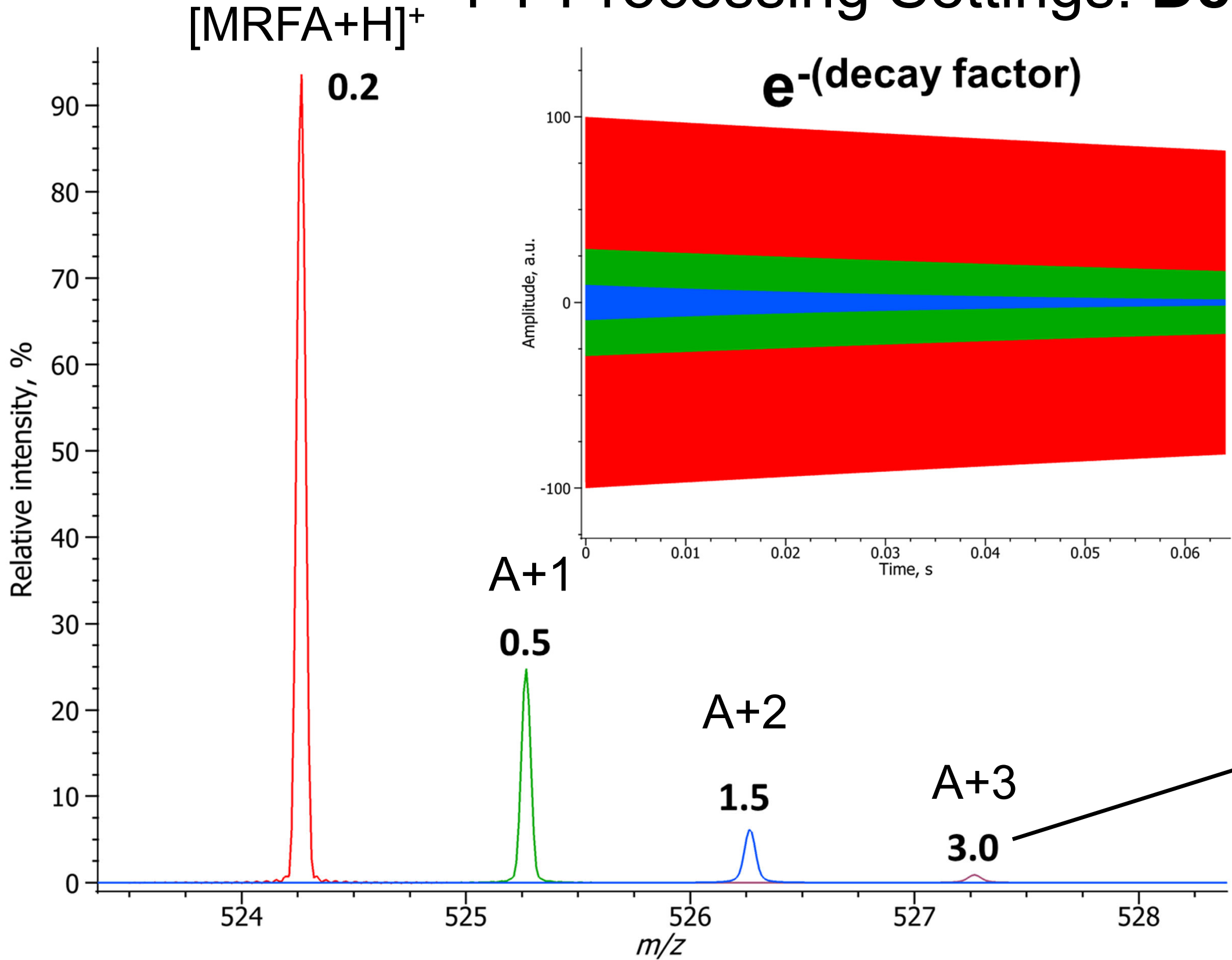


- Raw transient
- No decay

- Resulting transient with decay

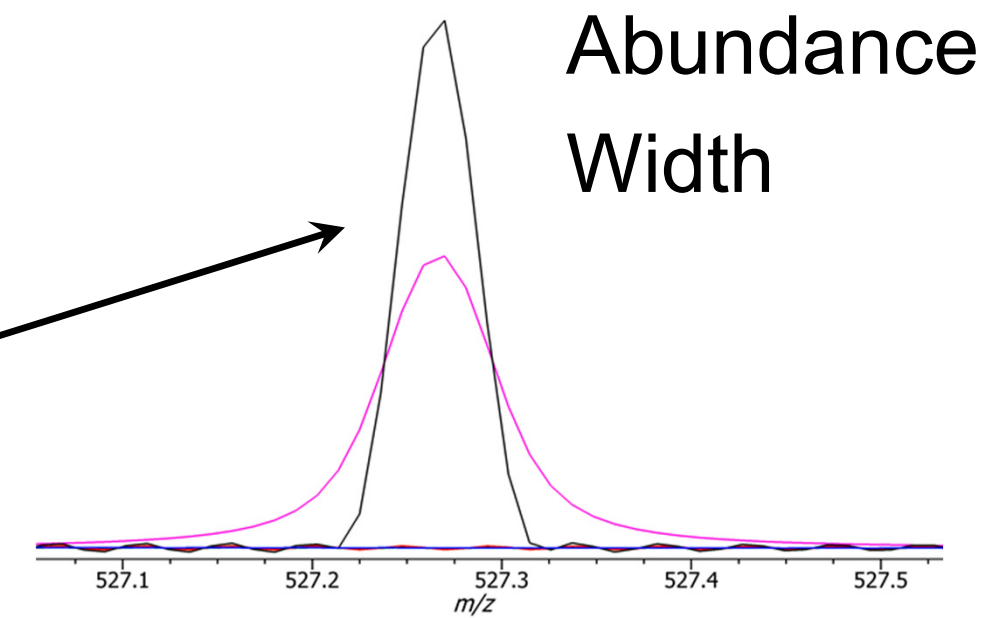
FT mode / apodization:	magnitude	None	
Zero-fills / sample rate:	2	4 MHz	
Noise / decay / phase:	0.000	0.80	0.0

# FT Processing Settings: Decay



- Example: MRFA peptide *in-silico* analysis with a Q Exactive Orbitrap™
- Decay factors for isotopologues are S/N dependent

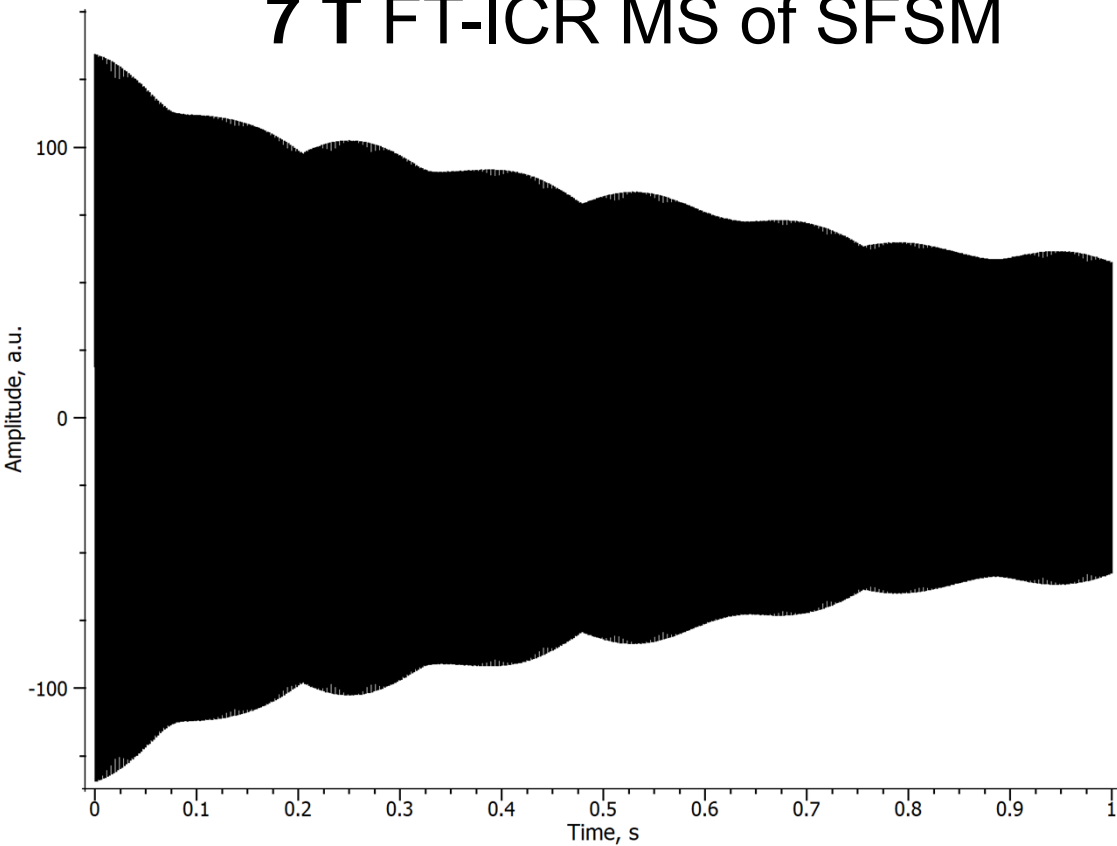
## Isotopic ratios errors





# FT Processing Settings: Apodization

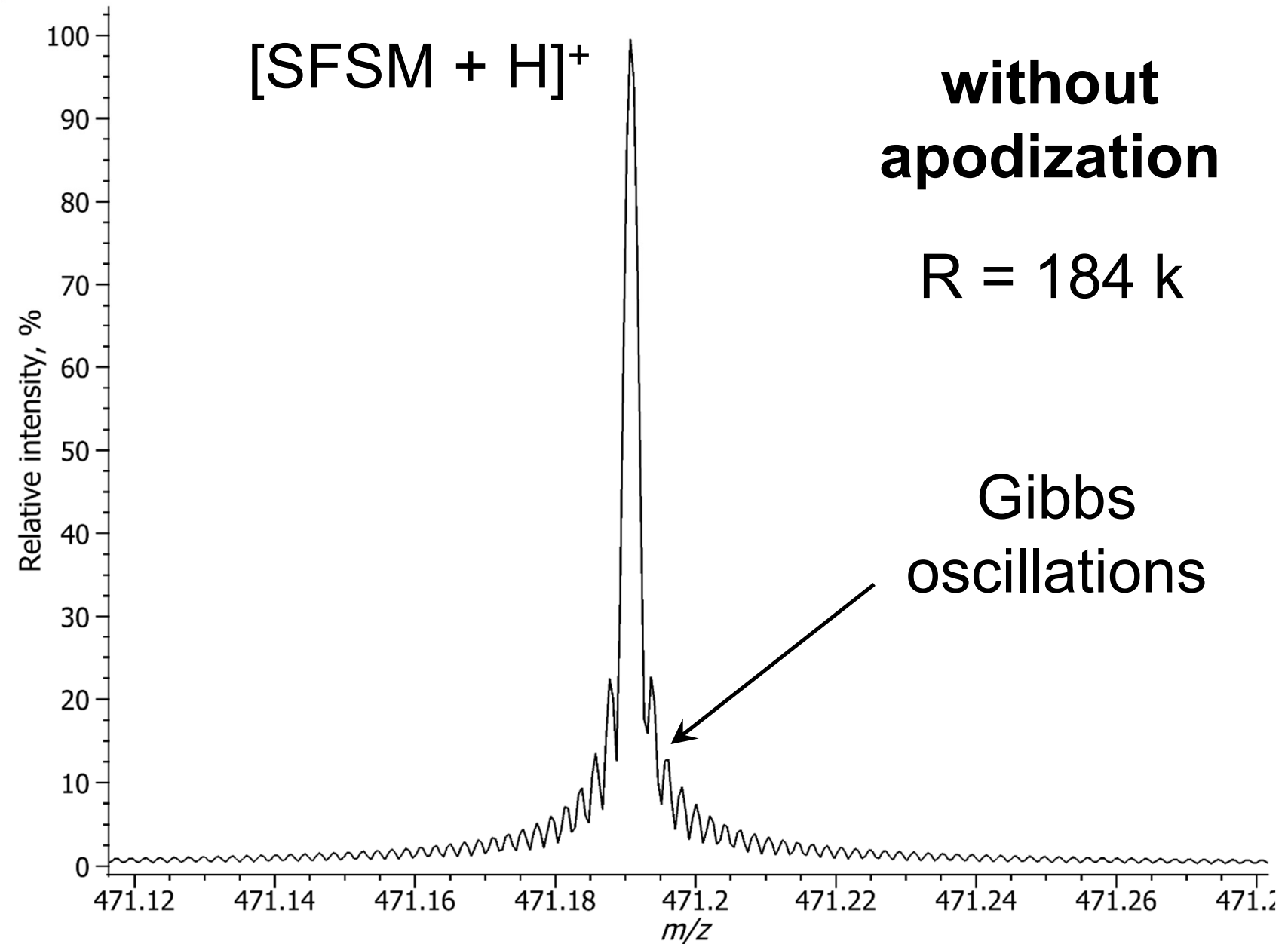
7 T FT-ICR MS of SF5M



mFT

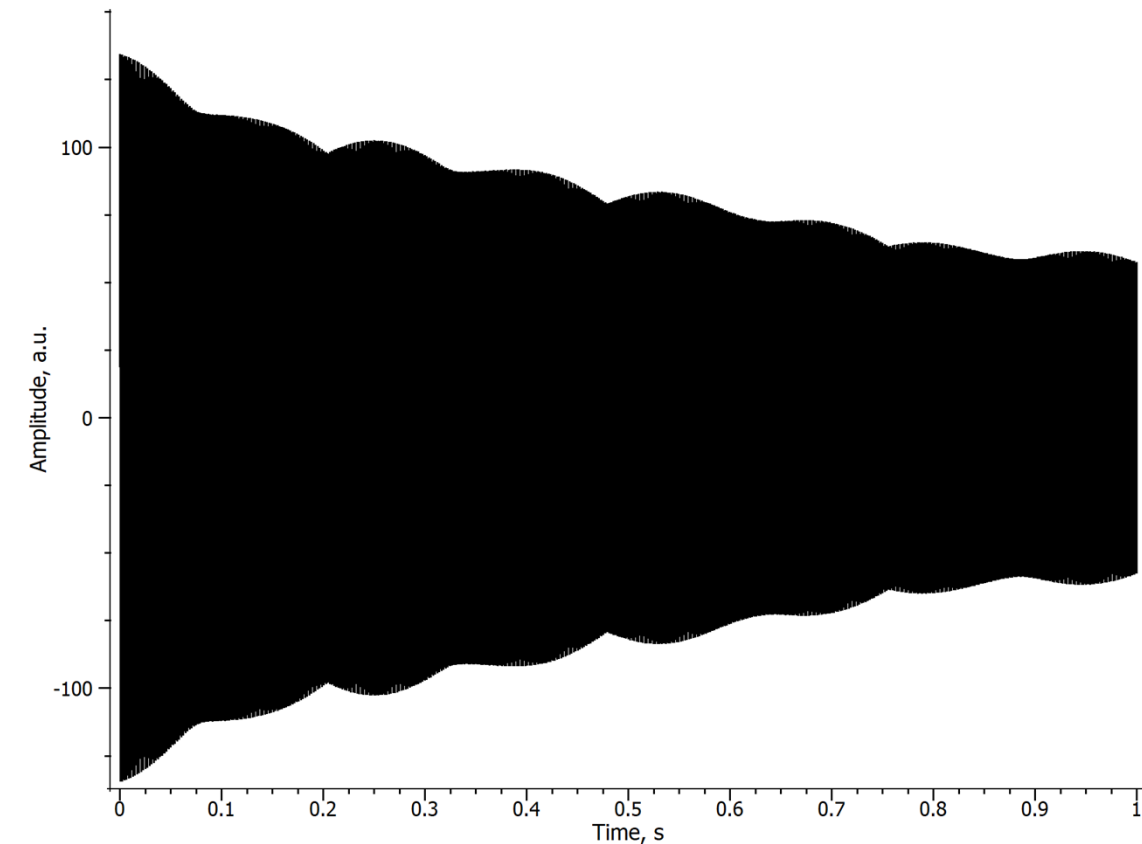


- Raw transient
- Squared off ends of transient cause multiple false peaks in spectrum

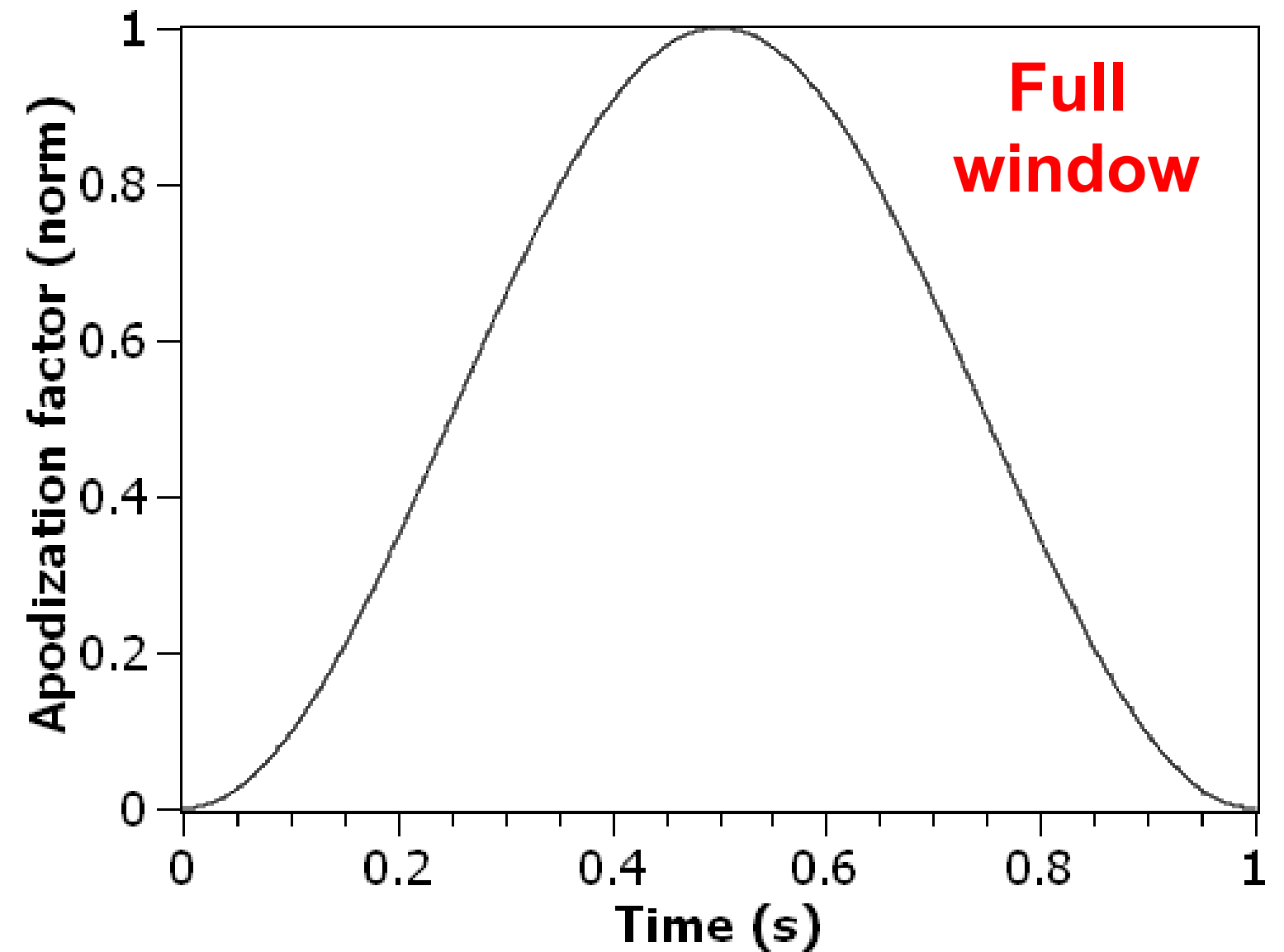


- Resulting mass spectrum
- Zoomed onto a single peak

# FT Processing Settings: Apodization



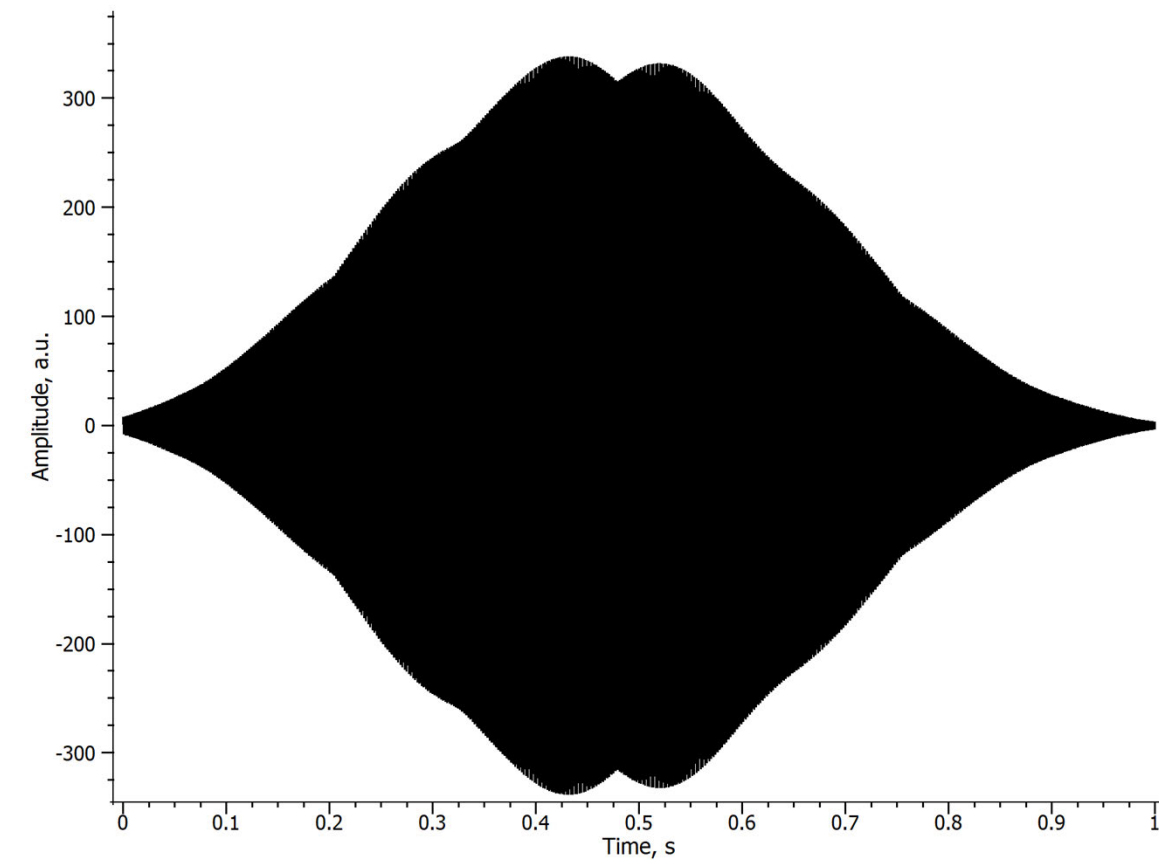
- Raw transient
- Squared off ends of transient cause multiple false peaks in spectrum



- Multiply transient by apodization function

# FT Processing Settings: Apodization

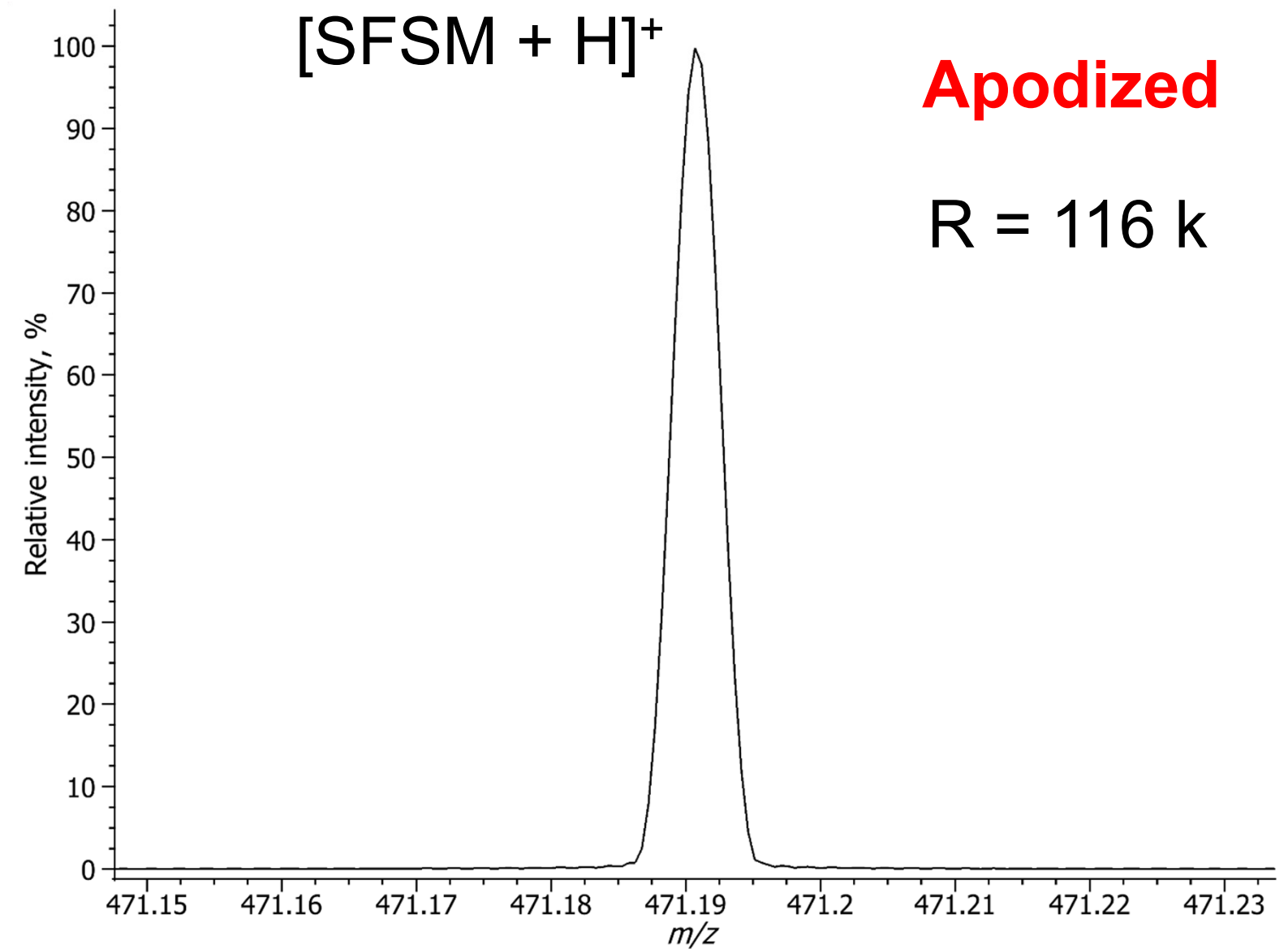
**Full window**



**mFT**

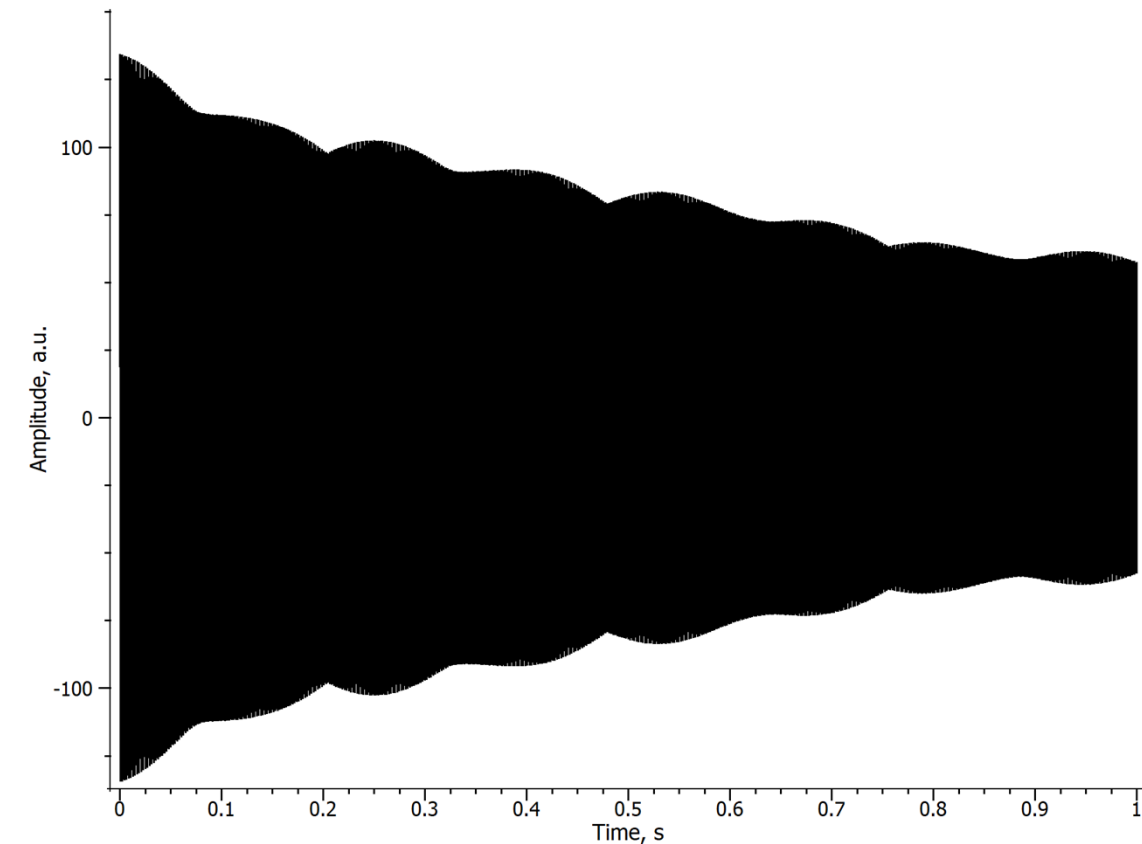


- Apodized transient
- Full window (Kaiser)
- No sharp edges
- No Gibbs oscillations

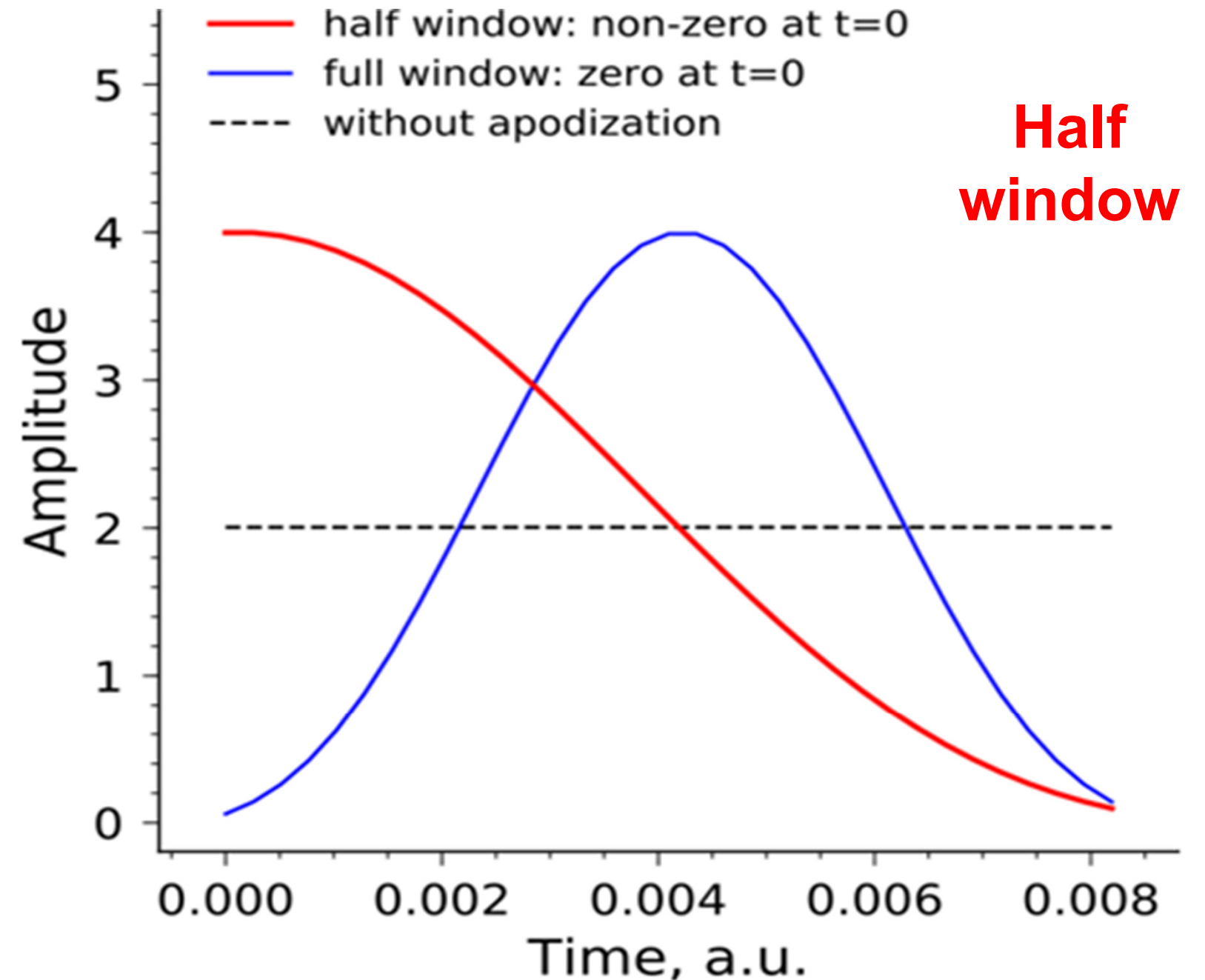


- But..
- Slight loss in resolution
- And loss in sensitivity

# FT Processing Settings: Apodization

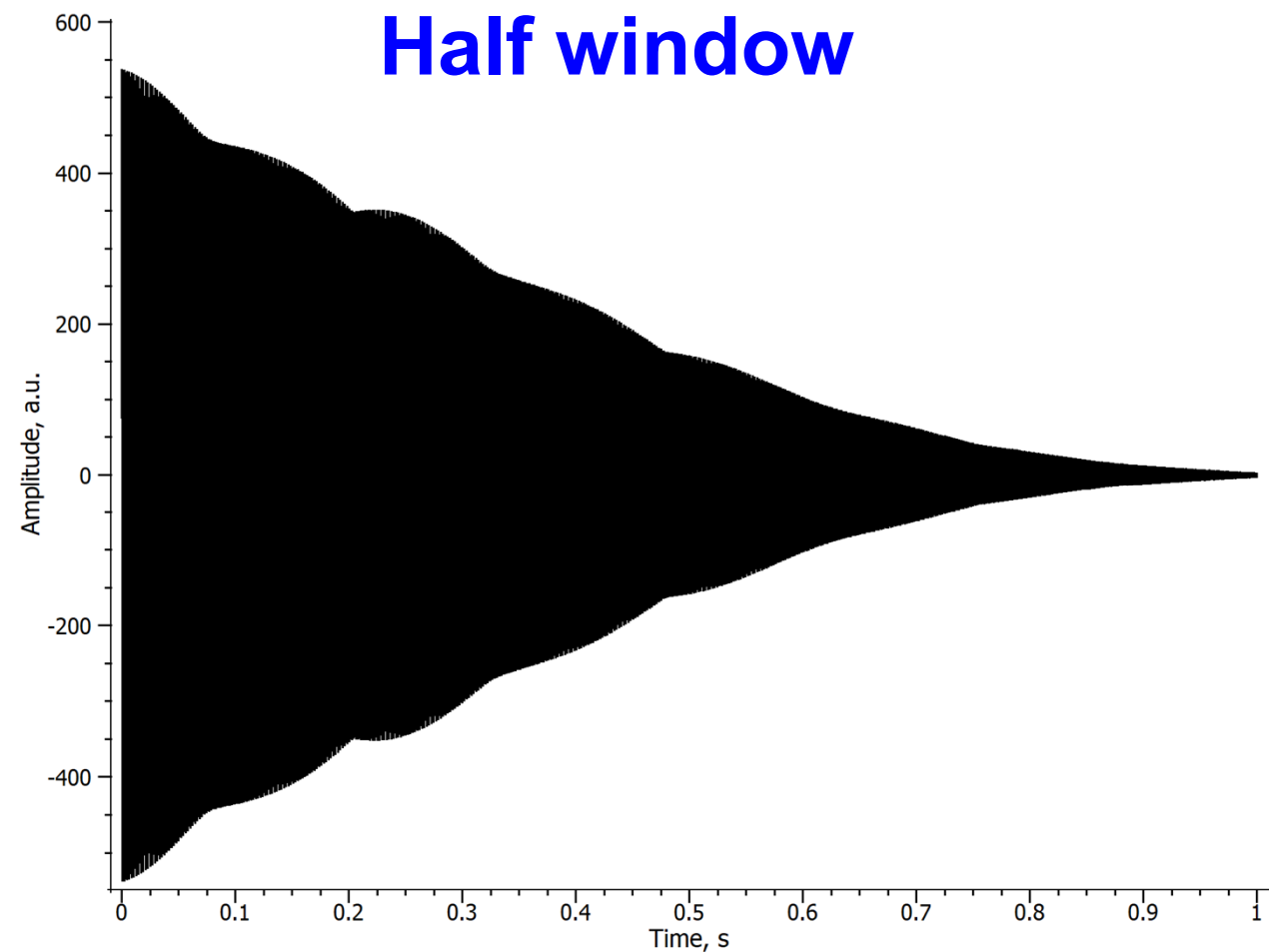


- Raw transient
- Squared off ends of transient cause multiple false peaks in spectrum

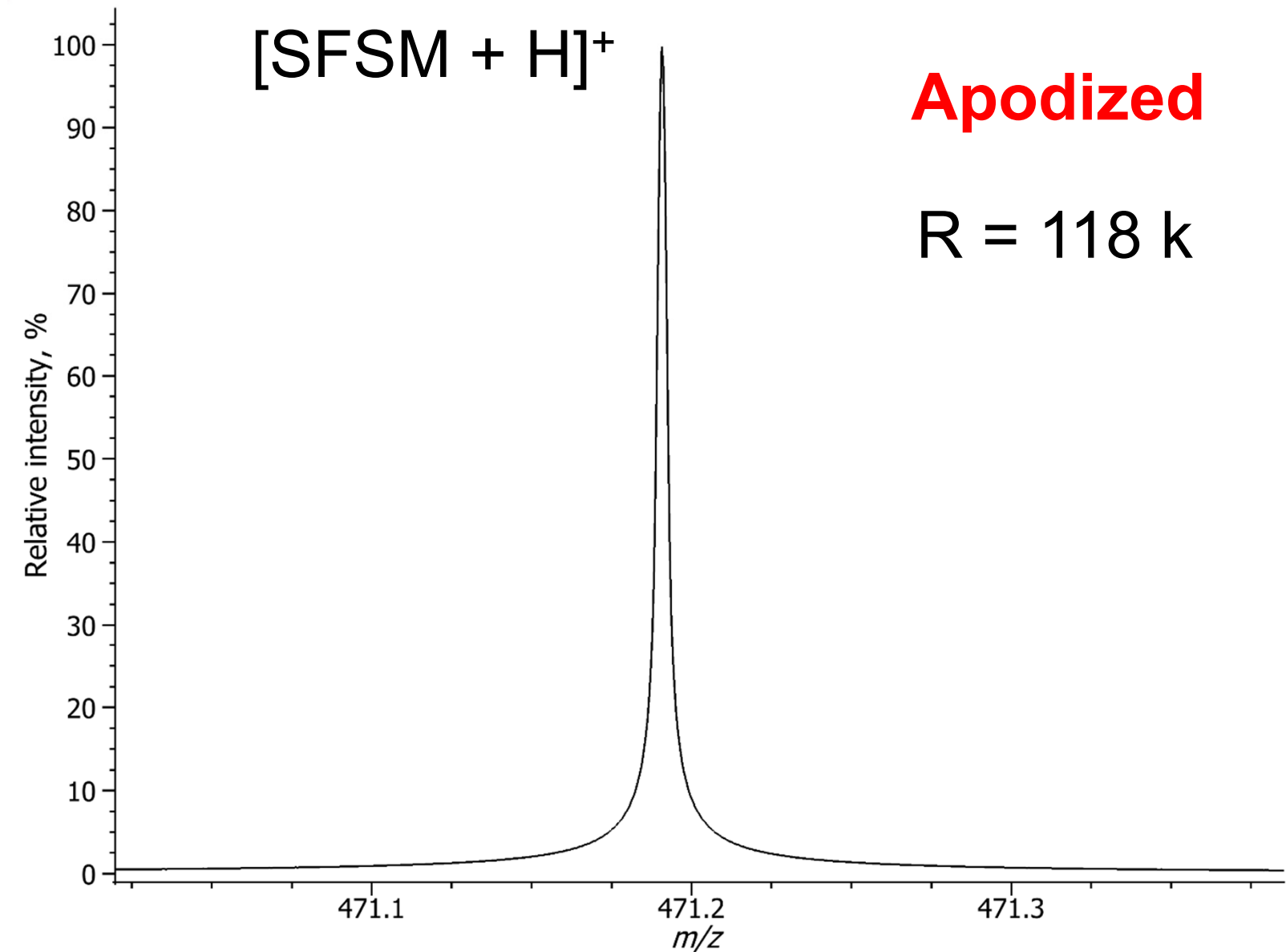


- Multiply transient by apodization function

# FT Processing Settings: Apodization



**mFT**

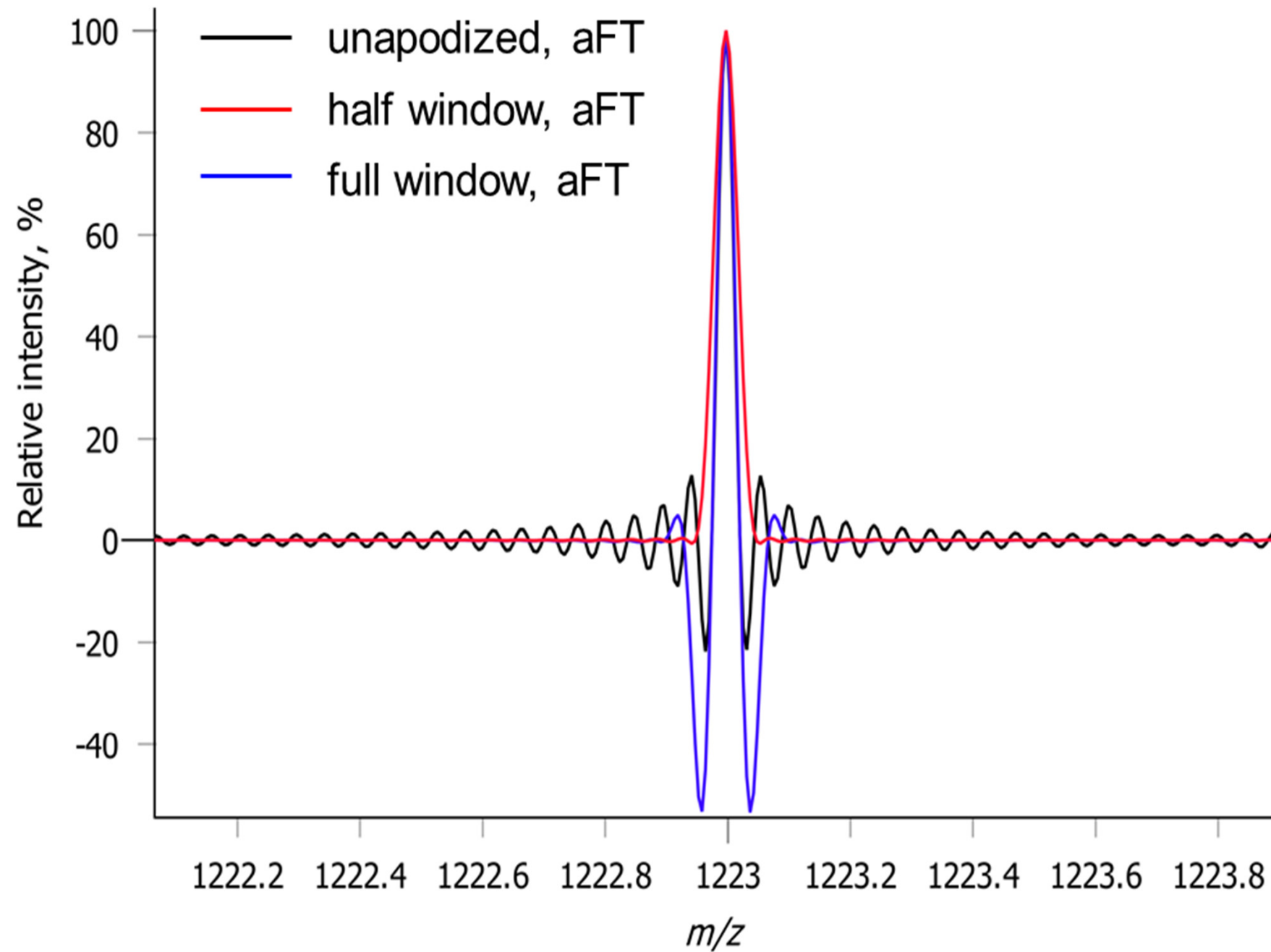


- Apodized transient
- Half window (Kaiser)
- No sharp edges
- No Gibbs oscillations

- But..
- Slight loss in resolution
- And loss in sensitivity

# FT Processing Settings: Apodization

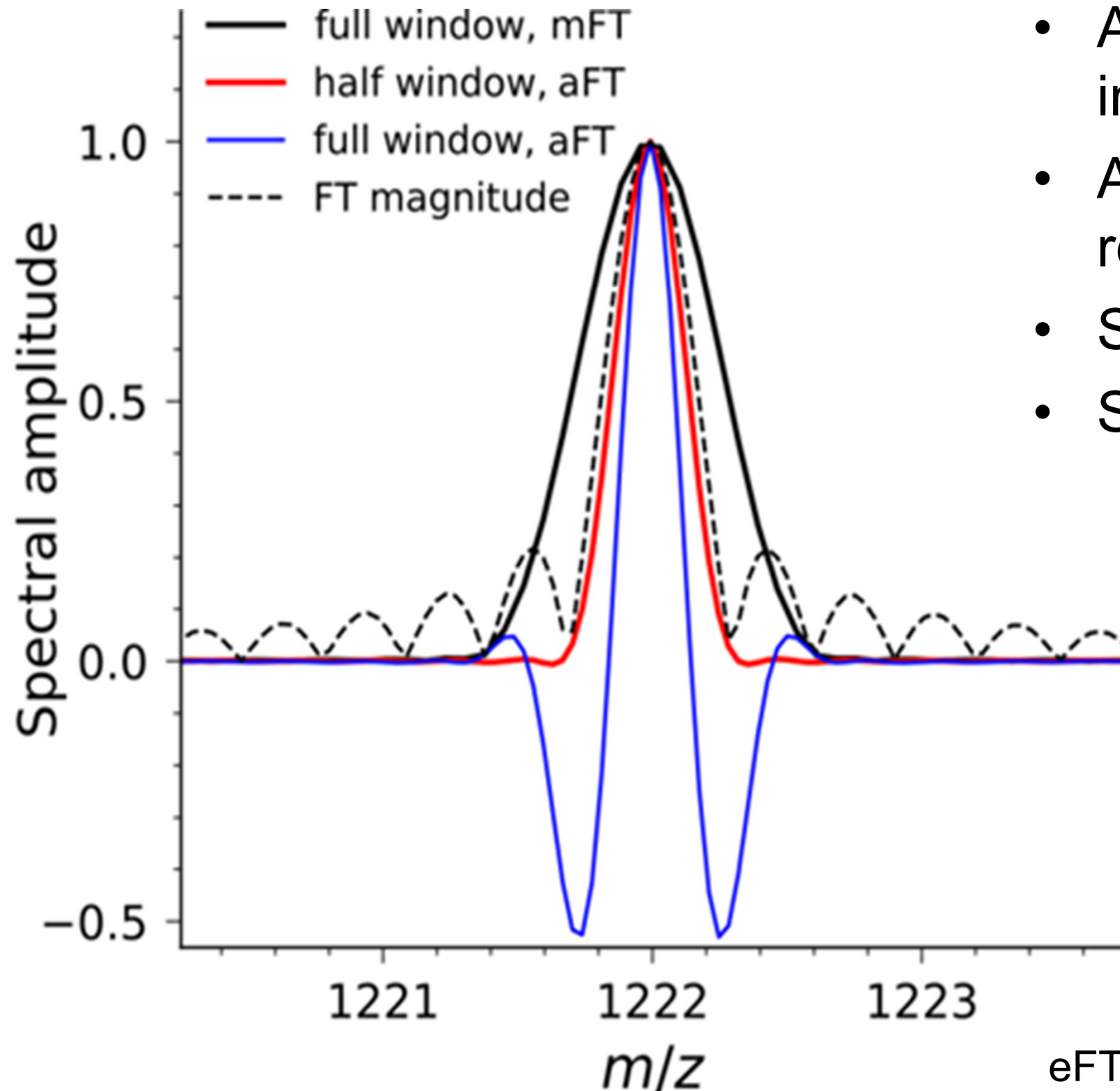
## Absorption mode FT (aFT)



- Apodization in aFT improves peak shape and removes artefacts, but
- Also slightly reduces peak abundance and resolution
- **Full** window apodization produces characteristic negative side lobes
- Technically it is harder to generate aFT mass spectra with **half** window apodization

For details see: <http://www.kilgourlab.com/absorption-mode-for-ft-ms/>

# FT Processing Settings: Apodization



- Apodization reduces resolution, but improves peak shape, reduces artefacts
- After apodization, mFT provides twice lower resolution than aFT
- Suggested apodization window for mFT: **full**
- Suggested apodization window for aFT: **half**



## eFT

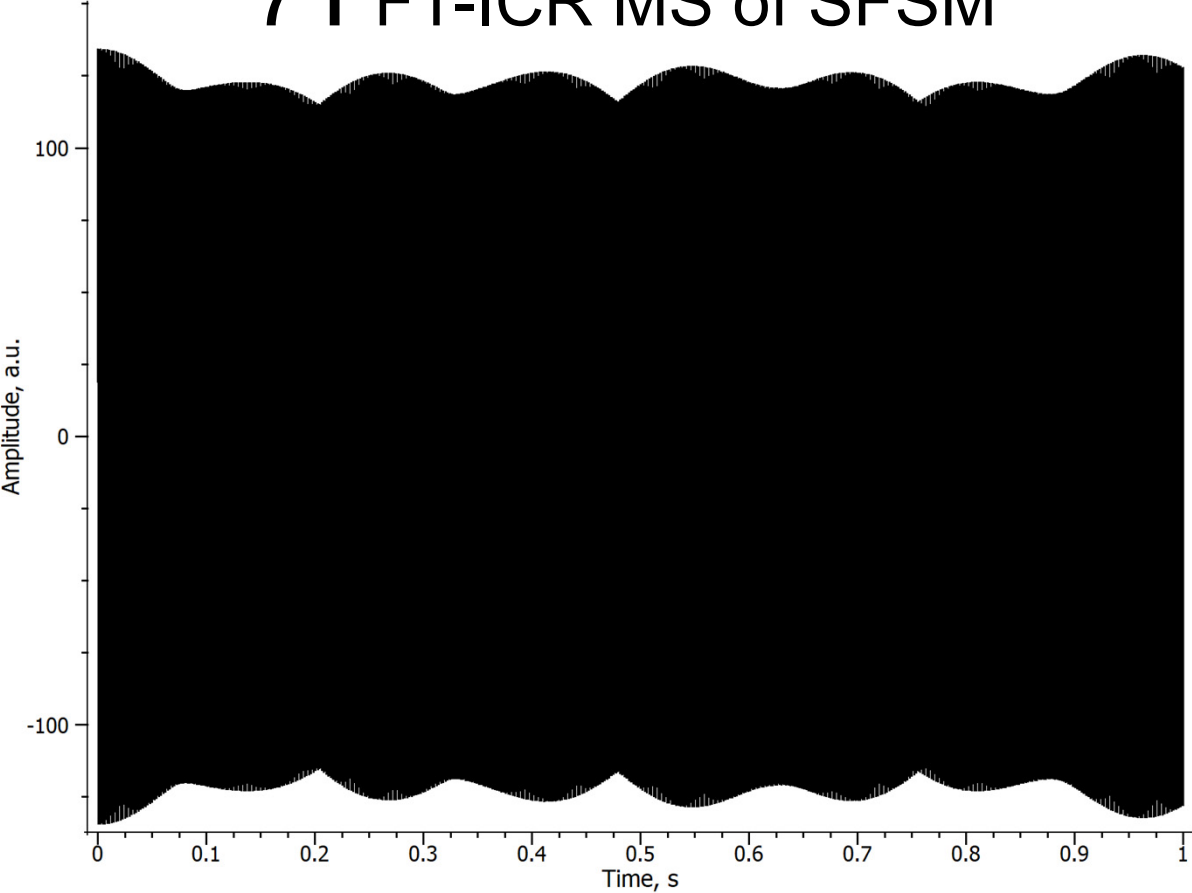
ThermoFisher  
SCIENTIFIC

- Enhanced FT (eFT) combines mFT/aFT
- Peak bottom (50%): **unapodized** mFT
- Peak top (50%): half window aFT
- Artefacts are smoothed/removed

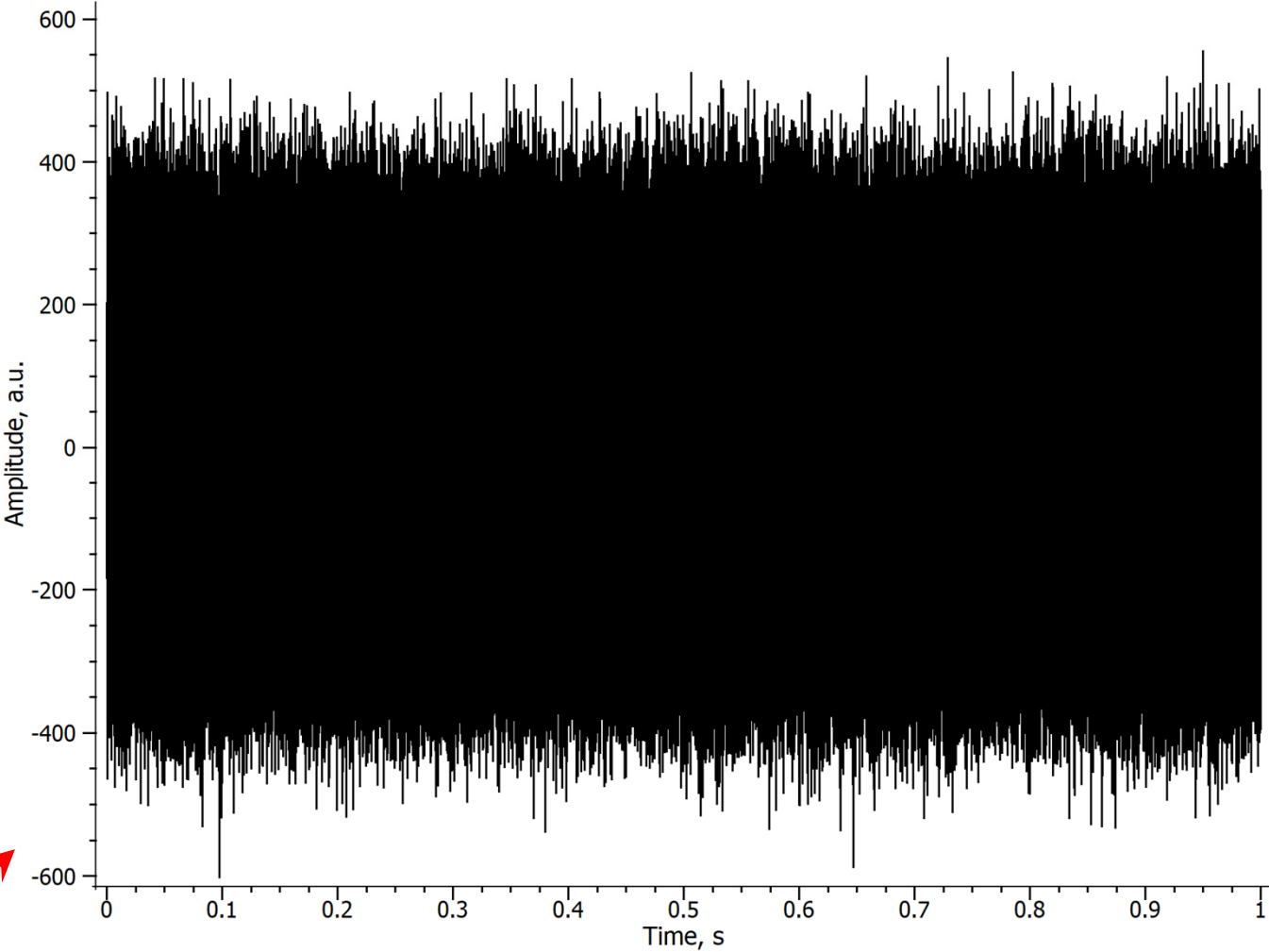
eFT principles: Lange, Makarov, *et al.* *IJMS* 369 (2014) 16–22

# FT Processing Settings: Noise

7 T FT-ICR MS of SF5M



+noise



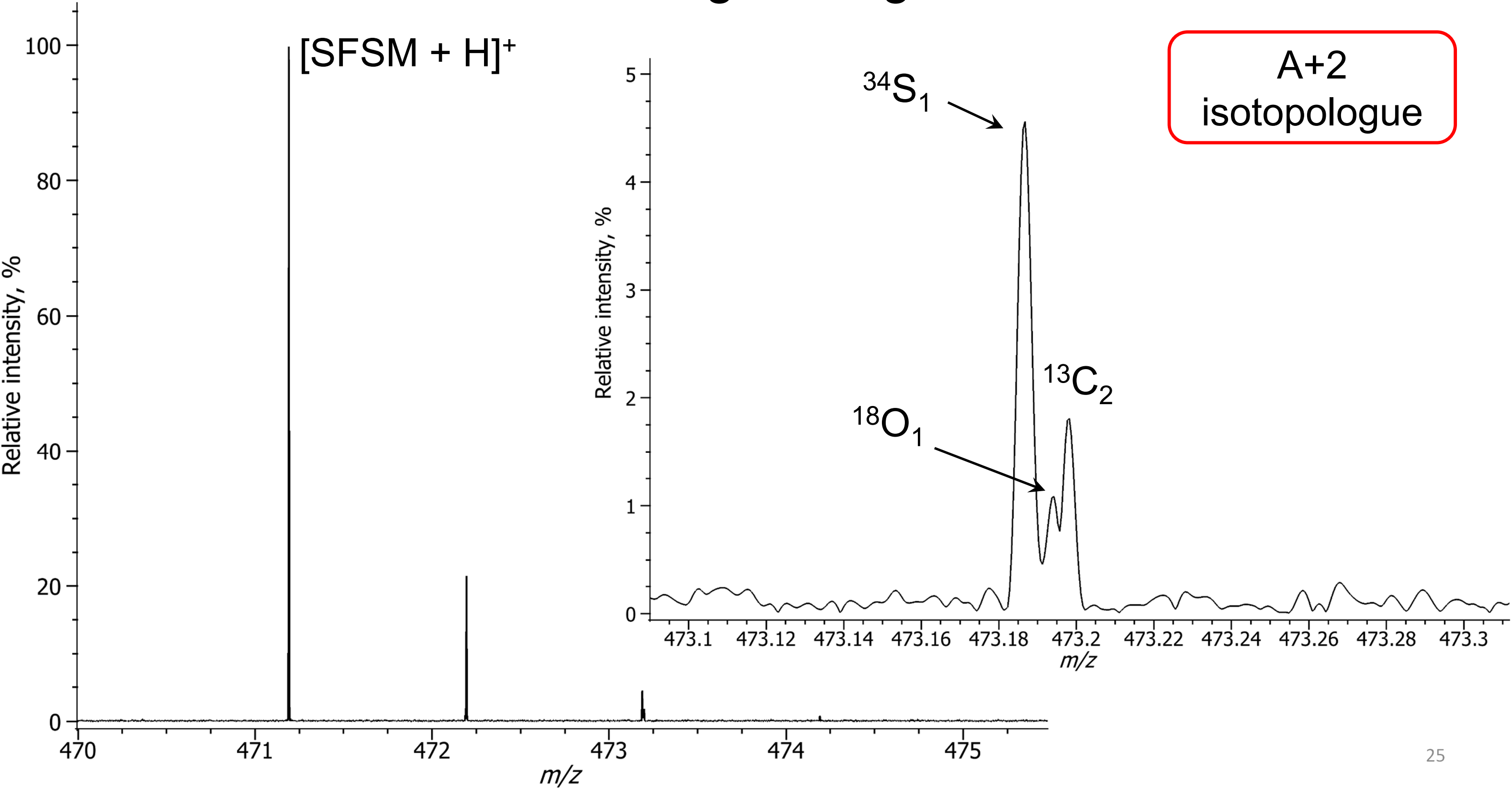
- Raw transient
- No noise

- Resulting transient with noise

FT mode / apodization:	magnitude	kaiser	
Zero-fills / sample rate:	2	4 MHz	
Noise / decay / phase:	1.000	0.00	0.0

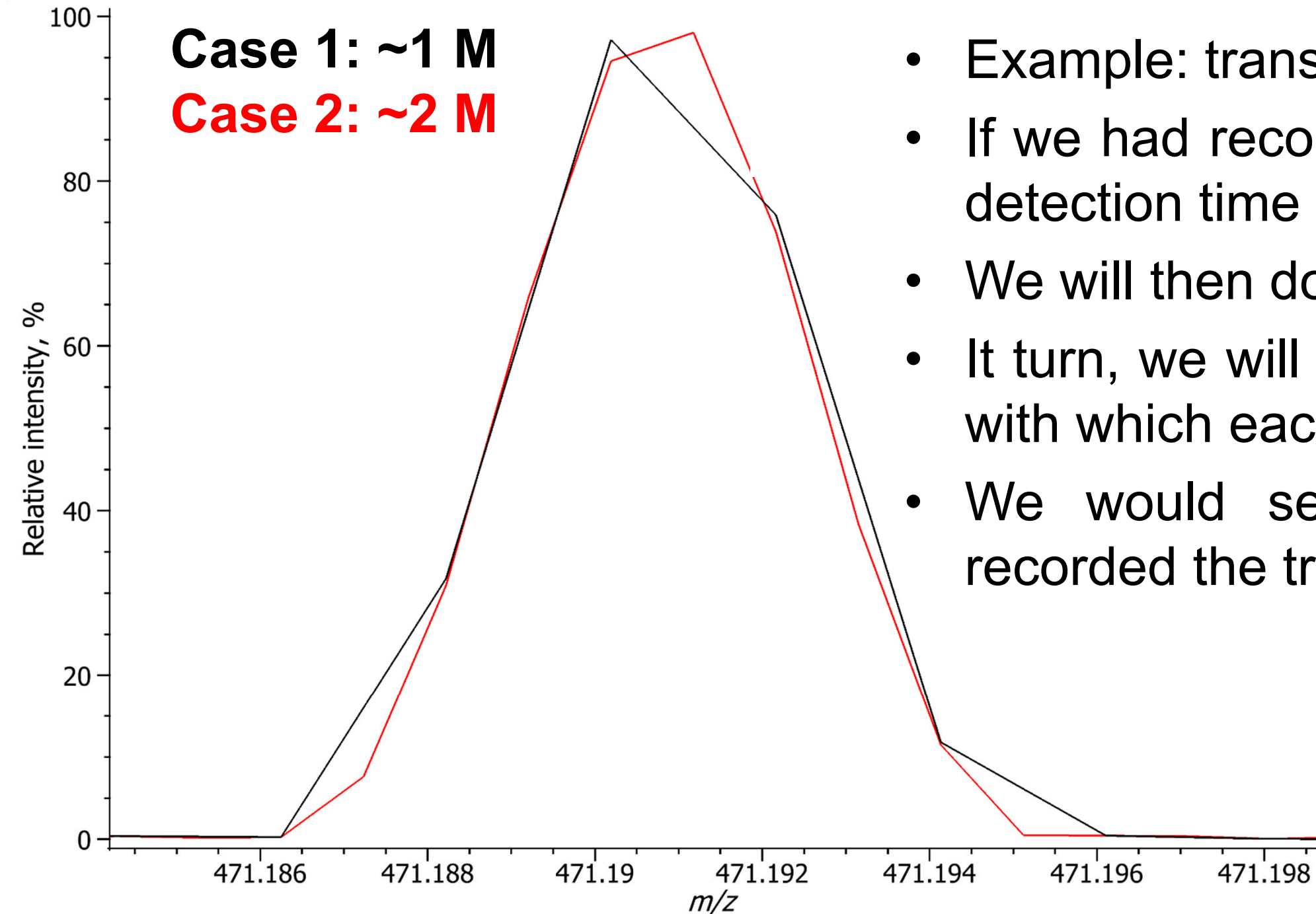


# FT Processing Settings: Noise

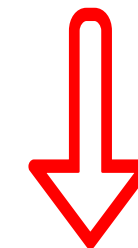


# FT Processing Settings: Zero-fills

- How to improve peak digitization for enhanced resolution and mass accuracy?



- Example: transient contains 1 M data points
- If we had recorded ~2 M points in the same ion detection time (transient length)
- We will then double the transient digitization rate
- It turn, we will double the number of data points with which each mass spectral peak is defined
- We would see the same effect if we had recorded the transient for twice as long



**An alternative:  
zero-fills (pads)**

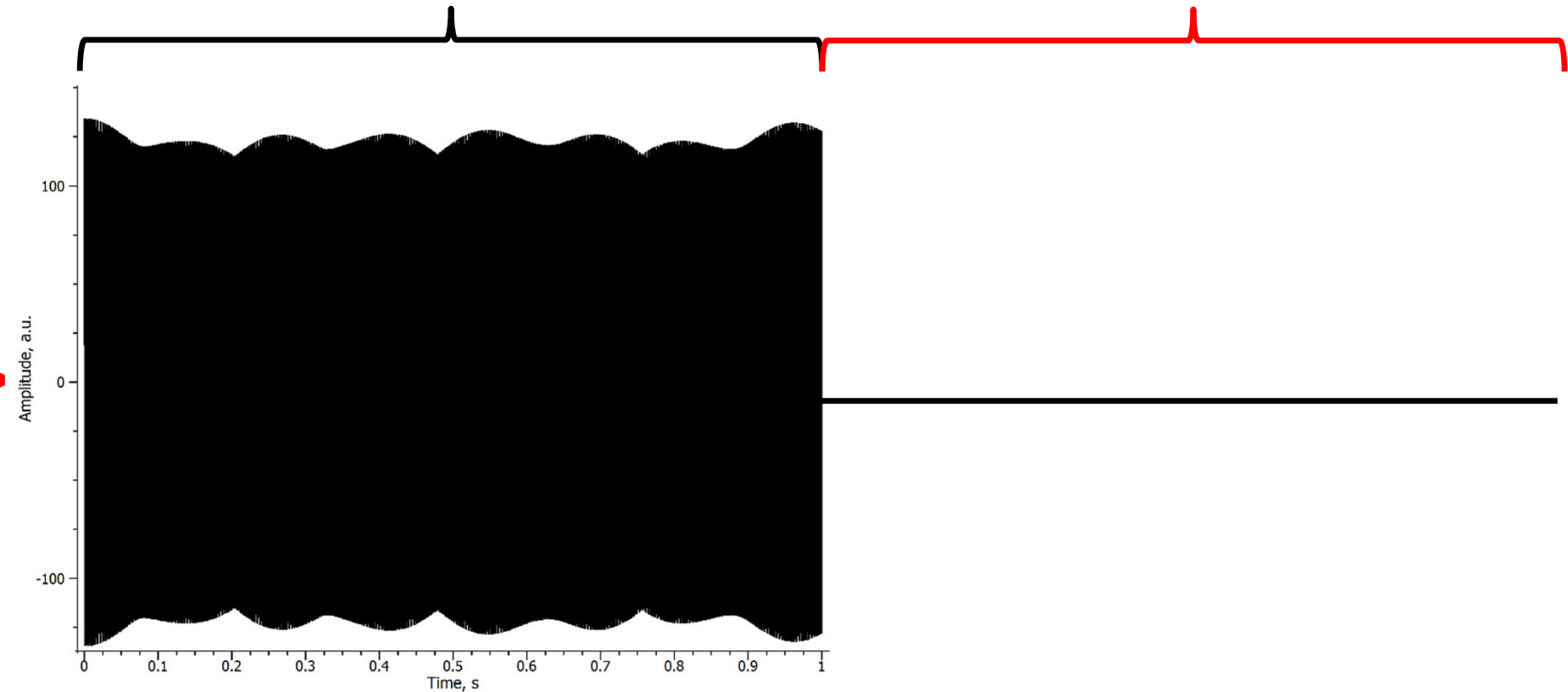
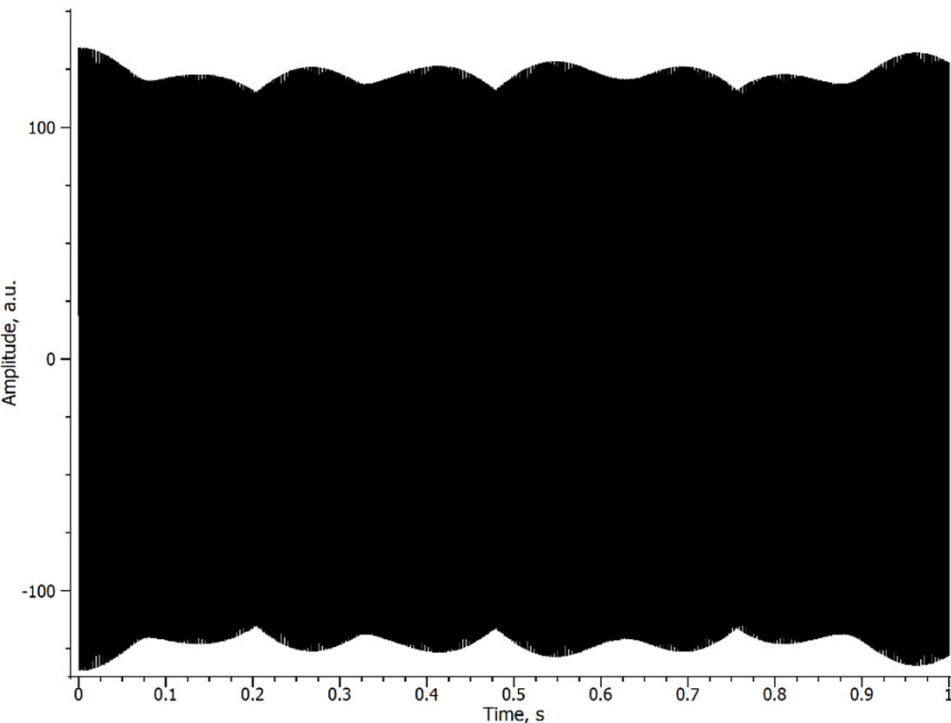
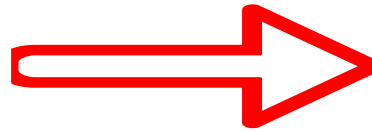
# FT Processing Settings: Zero-fills

7 T FT-ICR MS of SF5M

~1 M numbers

~1 M zeroes

add  
zeroes



- Raw transient

- Transient with one zero-fill (pad)
- Each zero-fill doubles the length of a transient (including prior zeroes)

FT mode / apodization:

magnitude

kaiser

Zero-fills / sample rate:

1

4 MHz

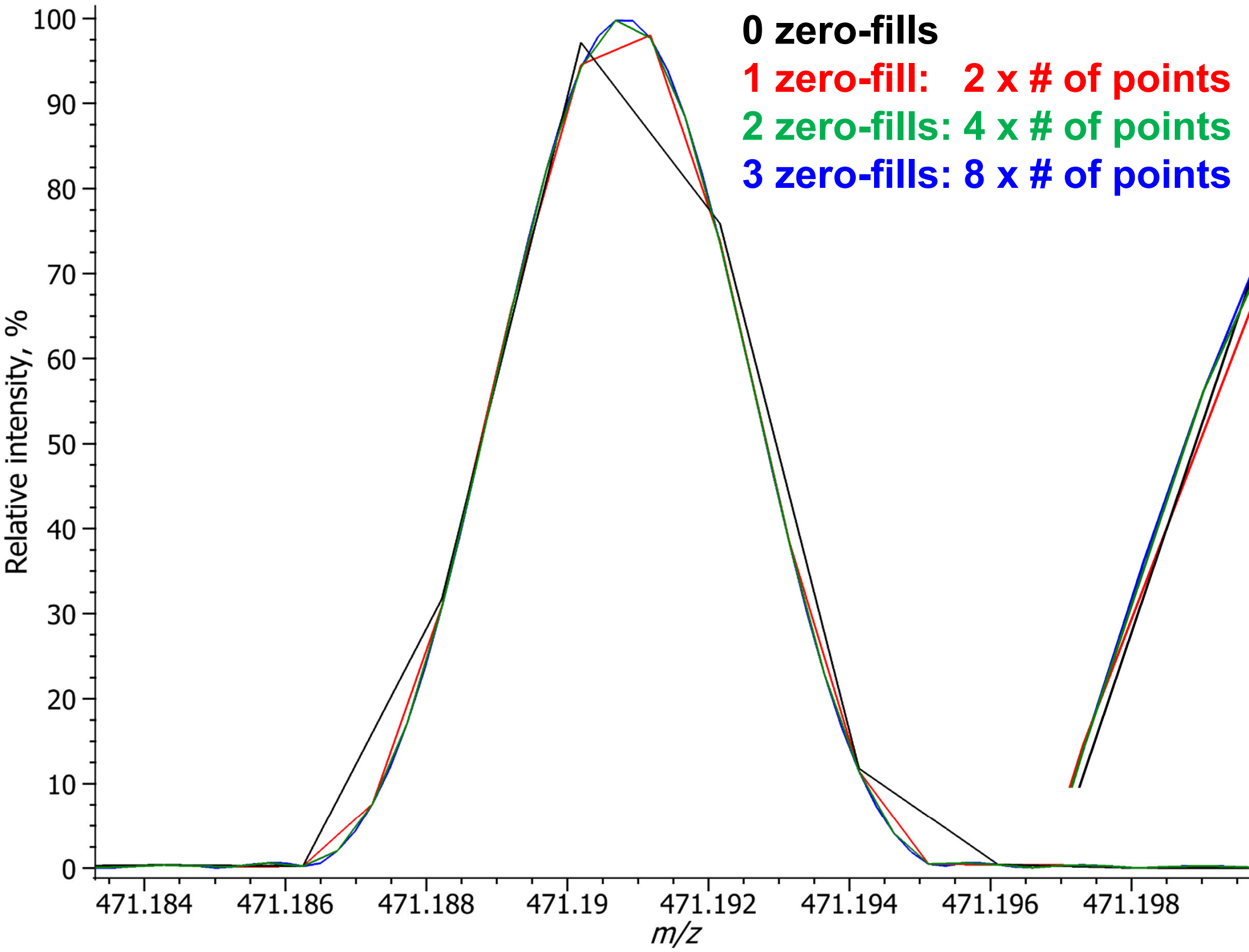
Noise / decay / phase:

1.000

0.00

0.0

# FT Processing Settings: Zero-fills



**Peak picking: a 3-point  
parabolic interpolation**

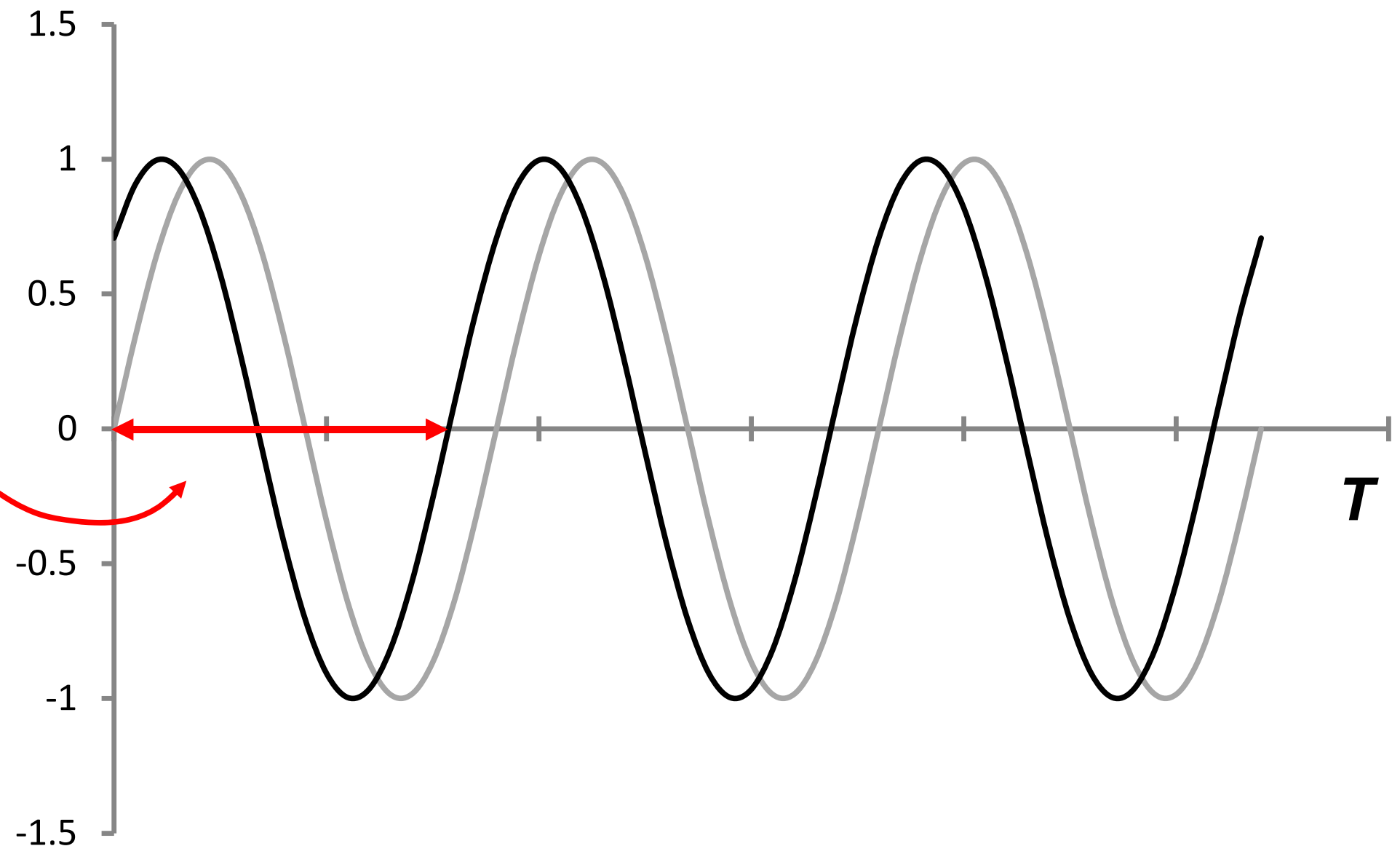
**Typically in FTMS:  
1-2 zero-fills**

# FT Processing Settings: Phase (Angle)

## Time-Domain Ion Signal: Transient

Three components to define a wave:

- Frequency
- Magnitude (measure of amplitude)
- **Phase (angle)**



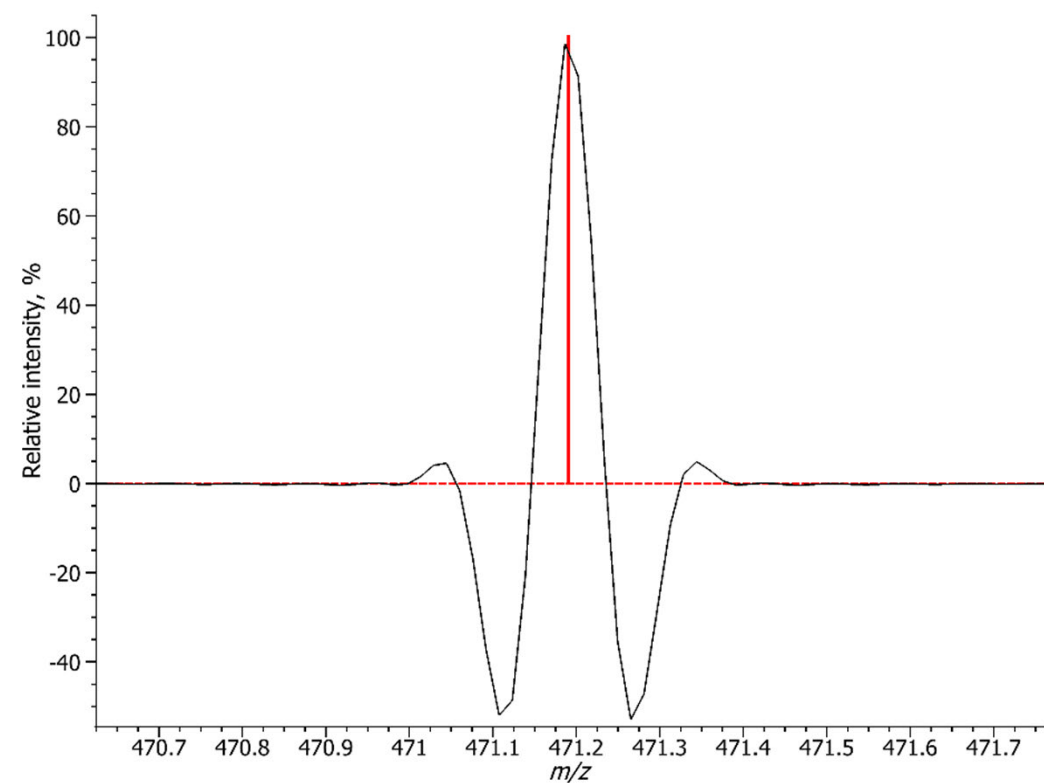
- example: two waves of the same frequency and amplitude, but different phase

For details see: <http://www.kilgourlab.com/absorption-mode-for-ft-ms/>

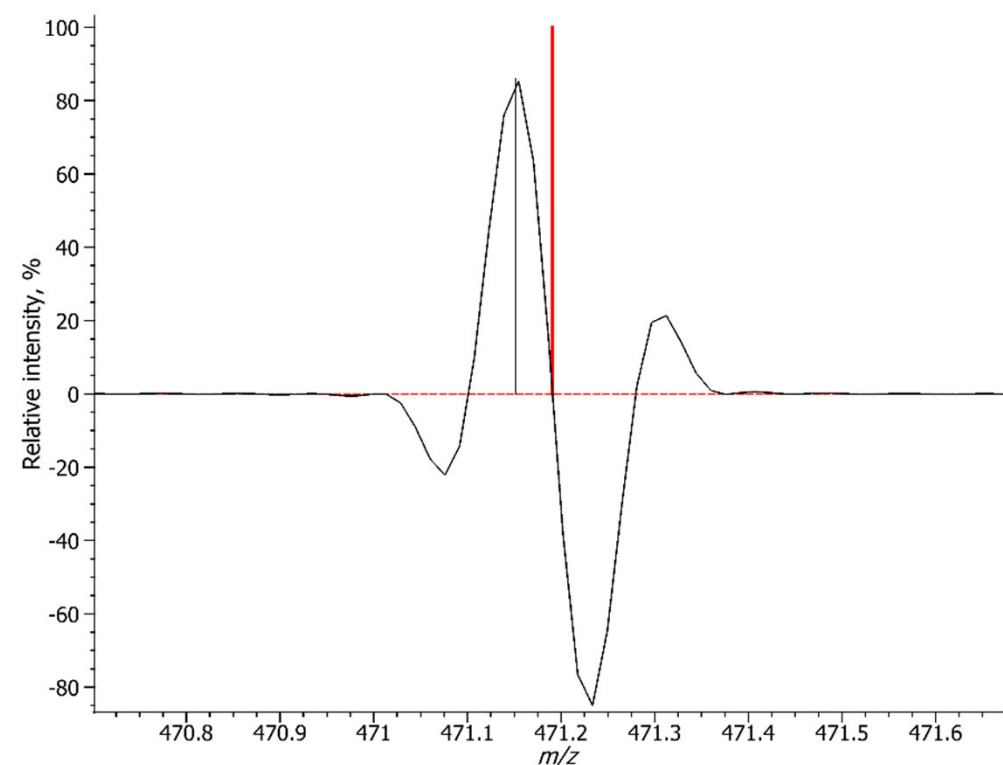
# FT Processing Settings: Phase (Angle)

- Example: 7 T FT-ICR MS of SFMS, absorption mode FT, full window (Kaiser)
- Phase shift results in peak artefacts: peak position ( $m/z$ ) and abundance
- Accurate phasing is crucial for artefact-free aFT mass spectra

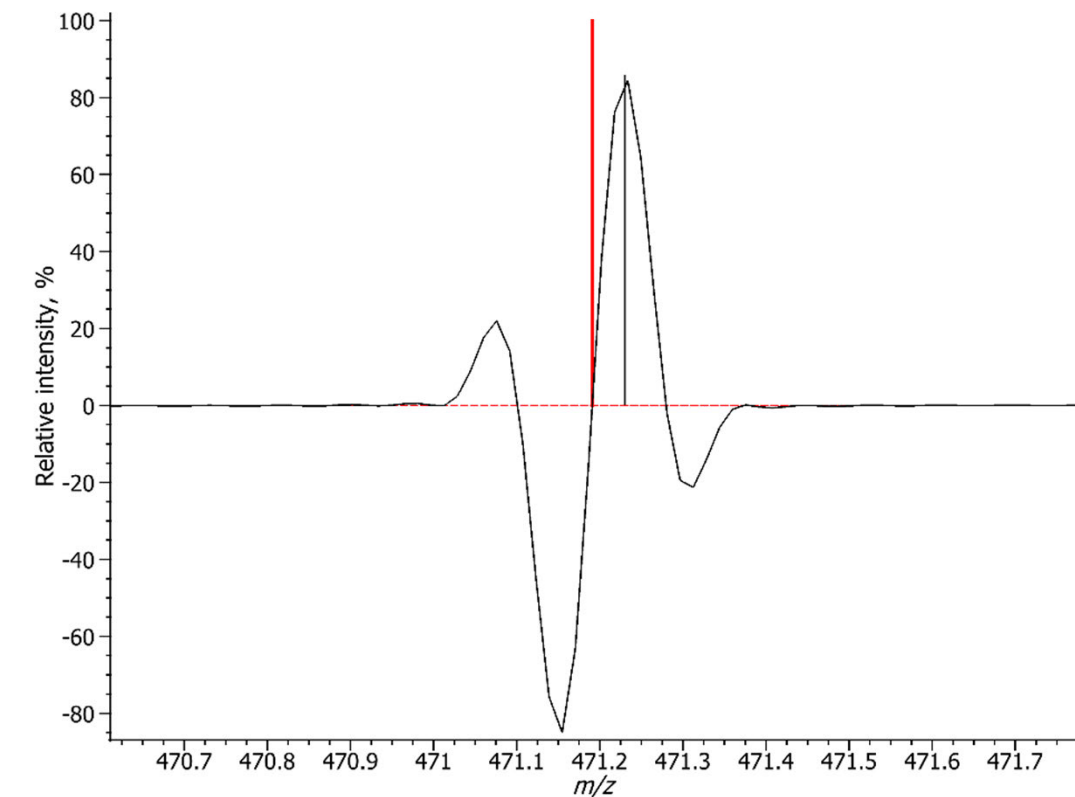
**Phase: 0 degrees**



**Phase: 90 degrees**



**Phase: 270 degrees**



For details see: <http://www.kilgourlab.com/absorption-mode-for-ft-ms/>