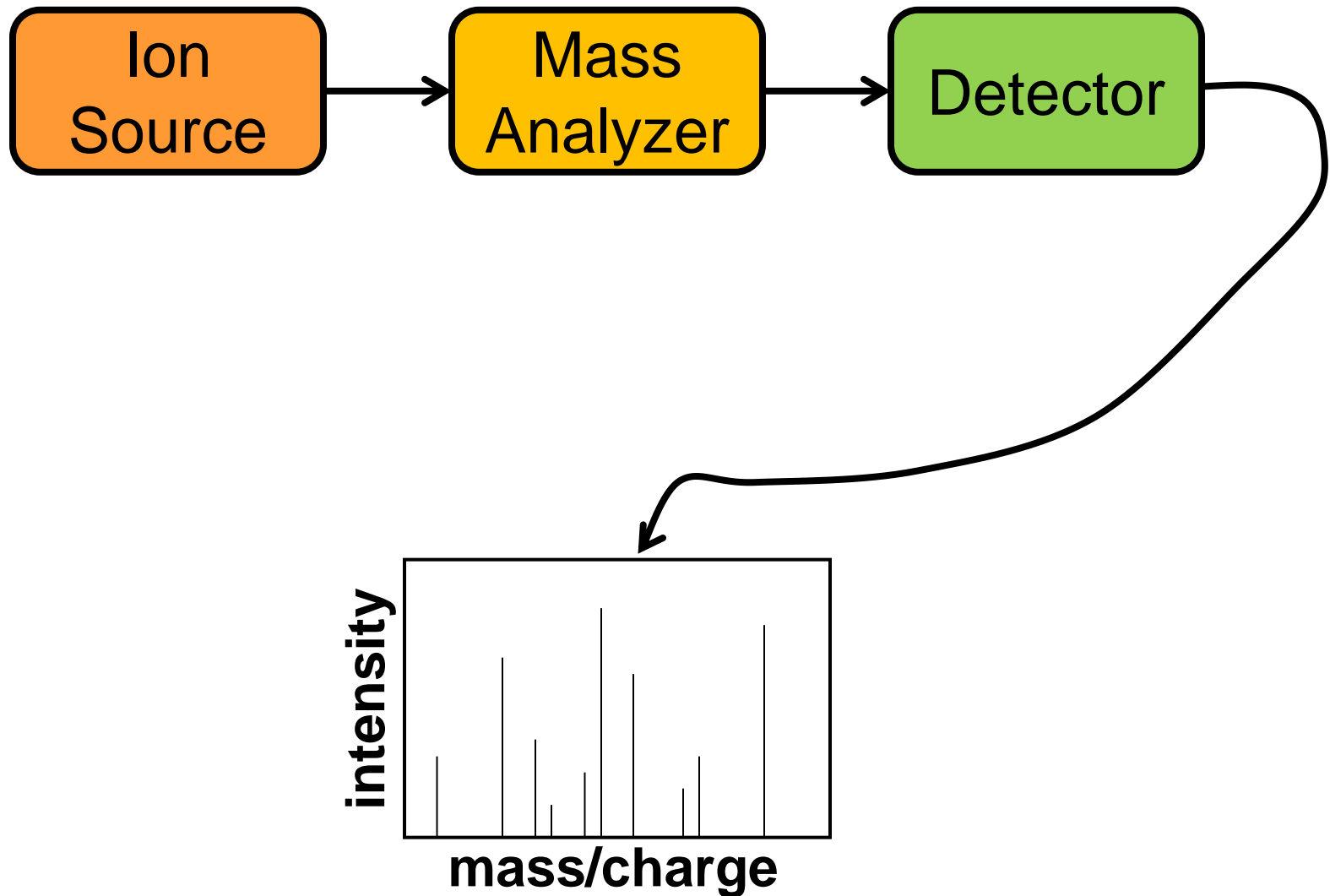
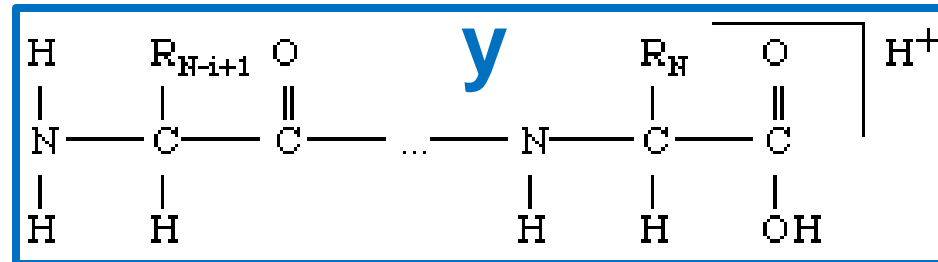
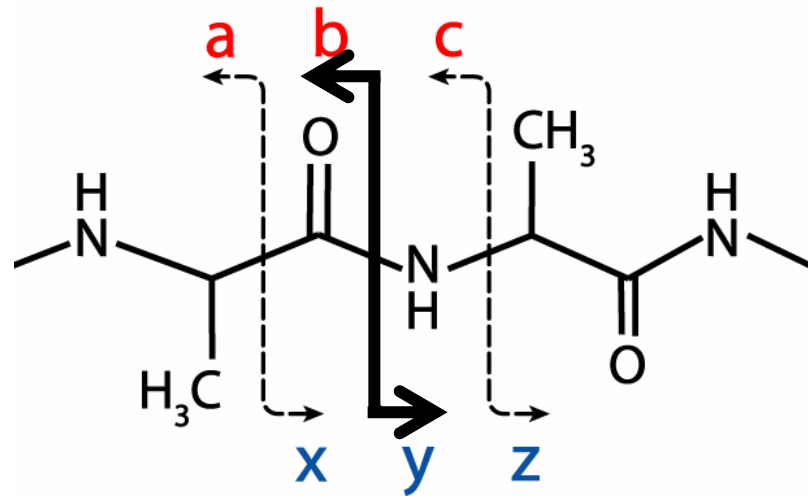
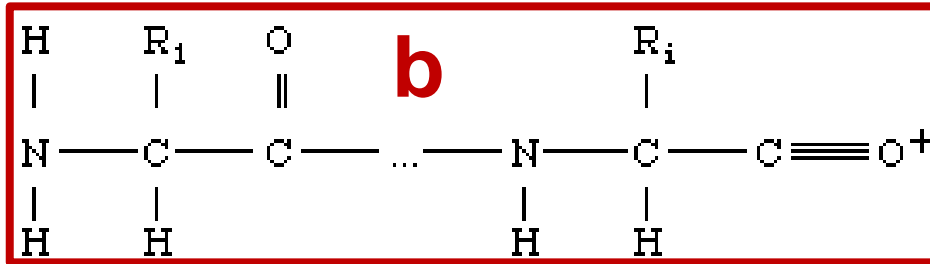


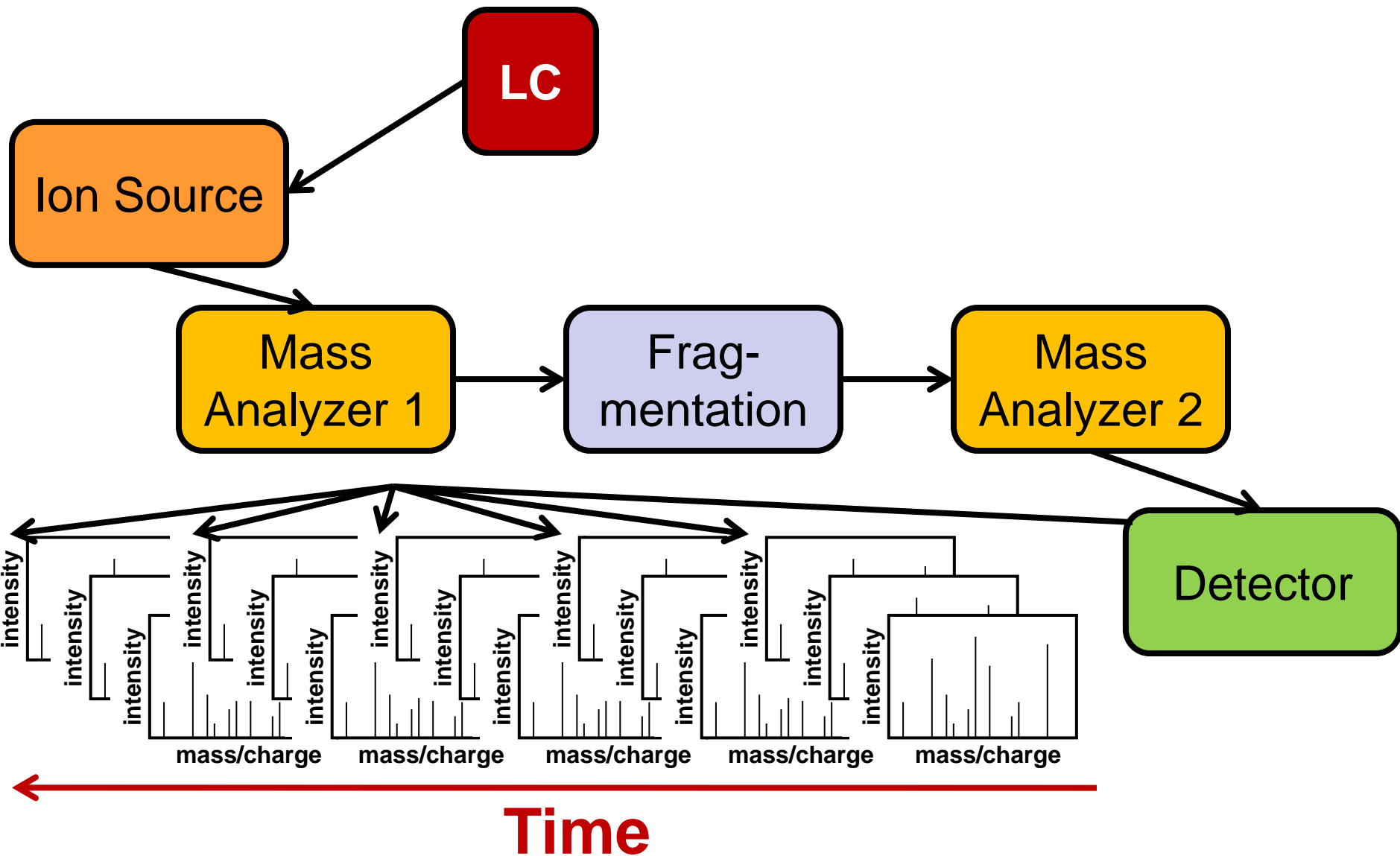
Proteomics Informatics - Overview of Mass spectrometry (Week 2)



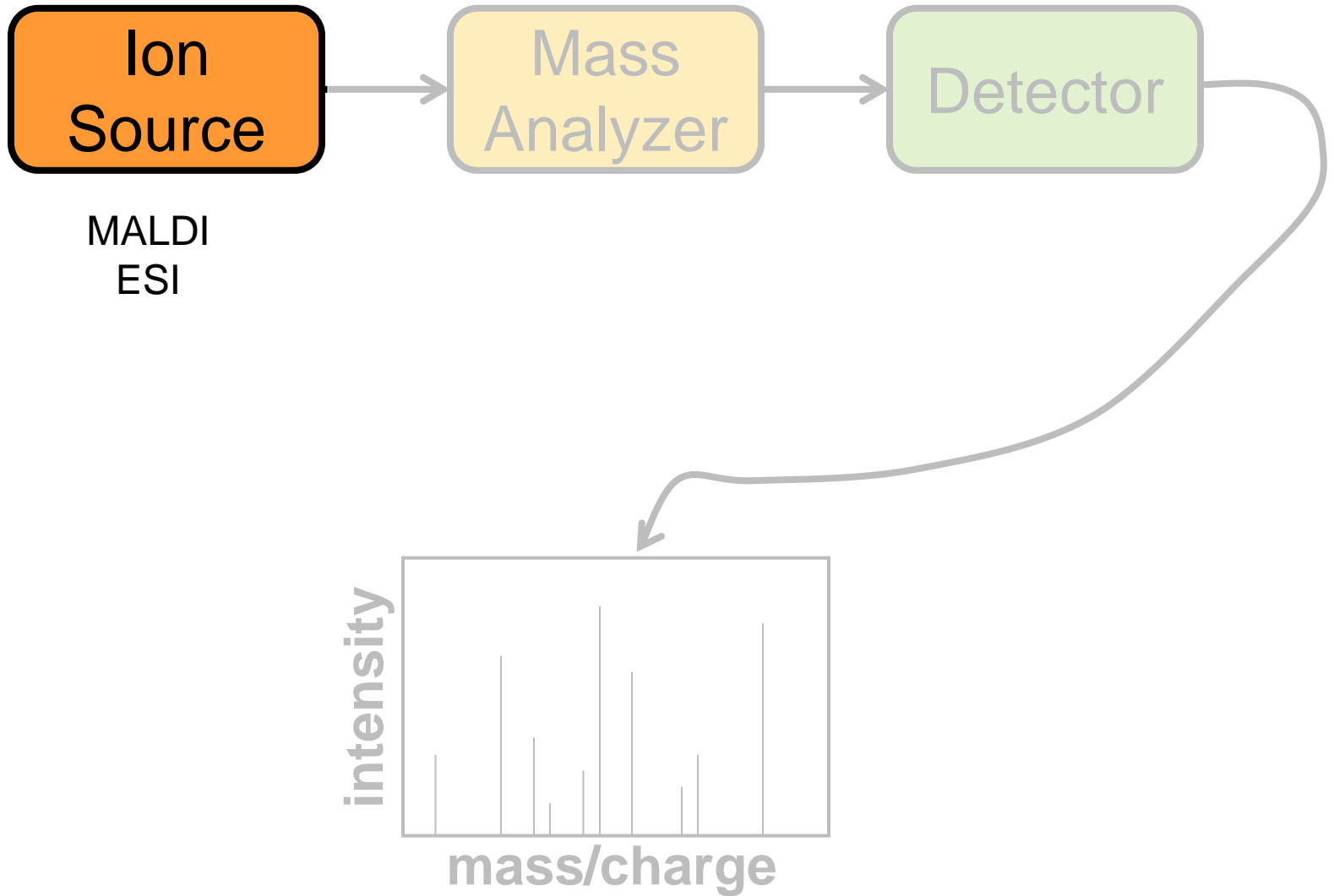
Peptide Fragmentation



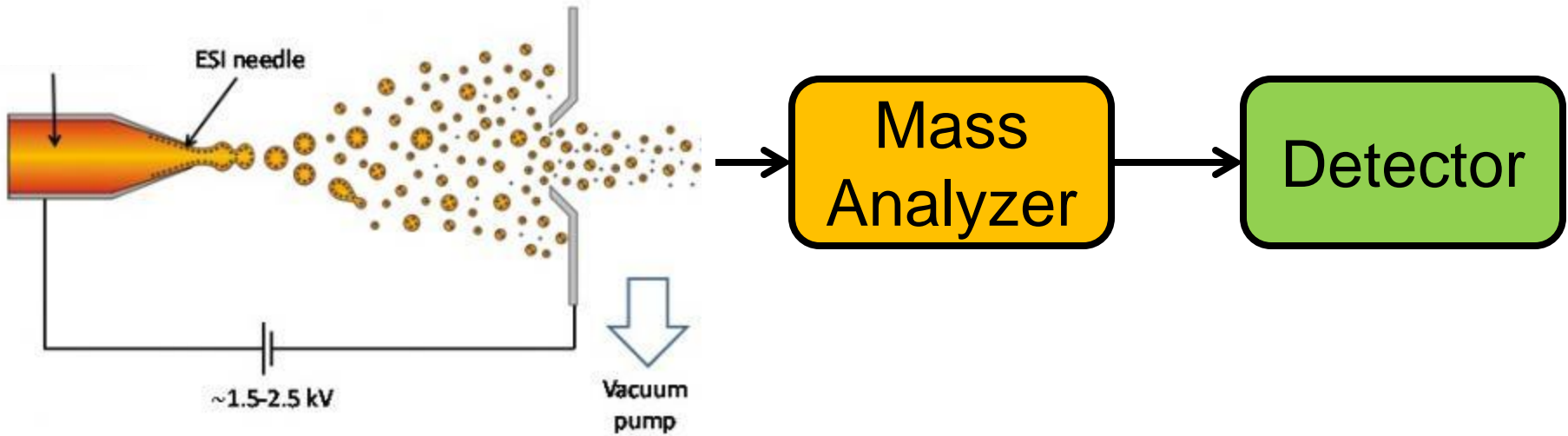
Liquid Chromatography (LC)-MS/MS



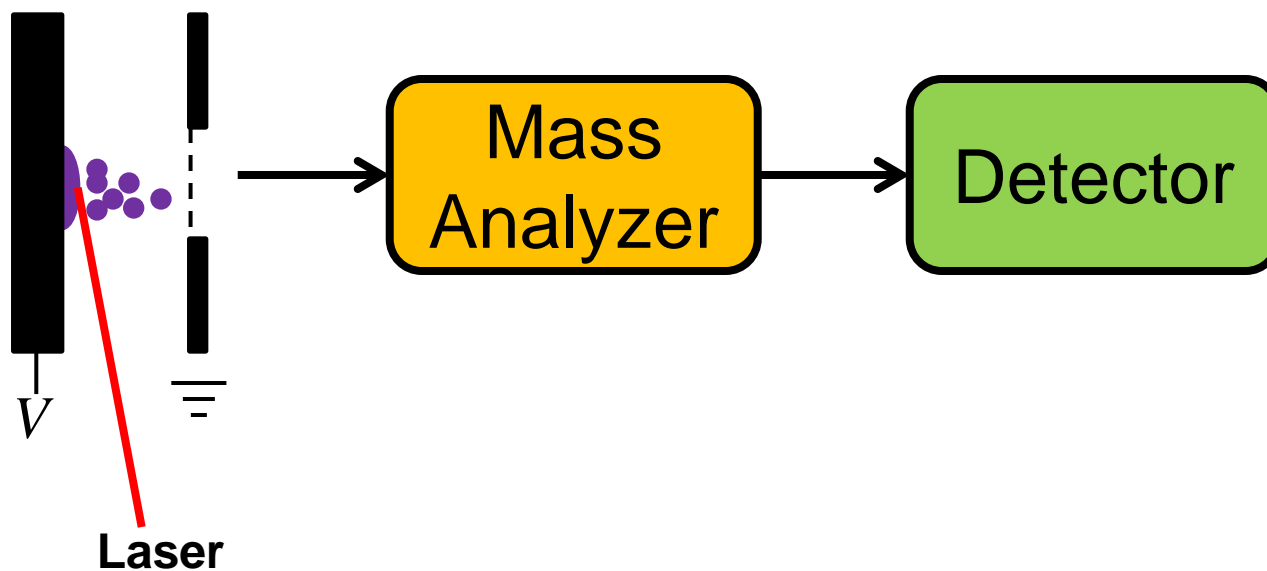
Ion Sources



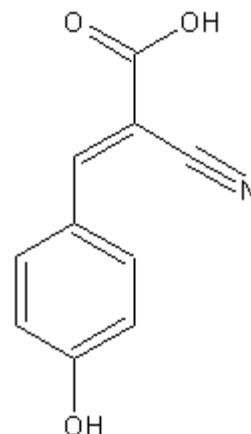
Electrospray



Matrix Assisted Laser Desorption Ionization (MALDI)

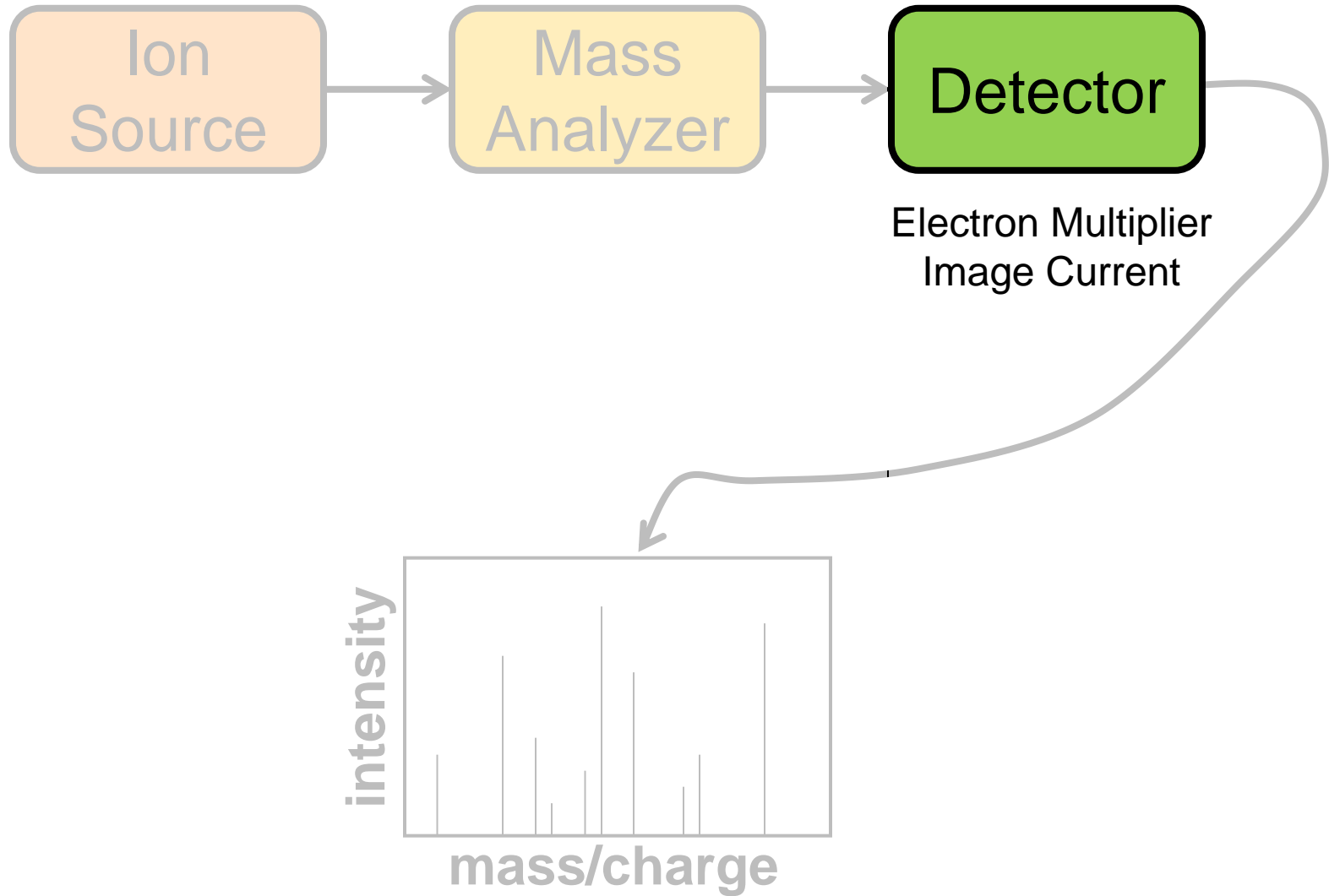


Matrix



alpha-cyano-4-hydroxycinnamic acid

Detectors



Electron Multiplier Detector

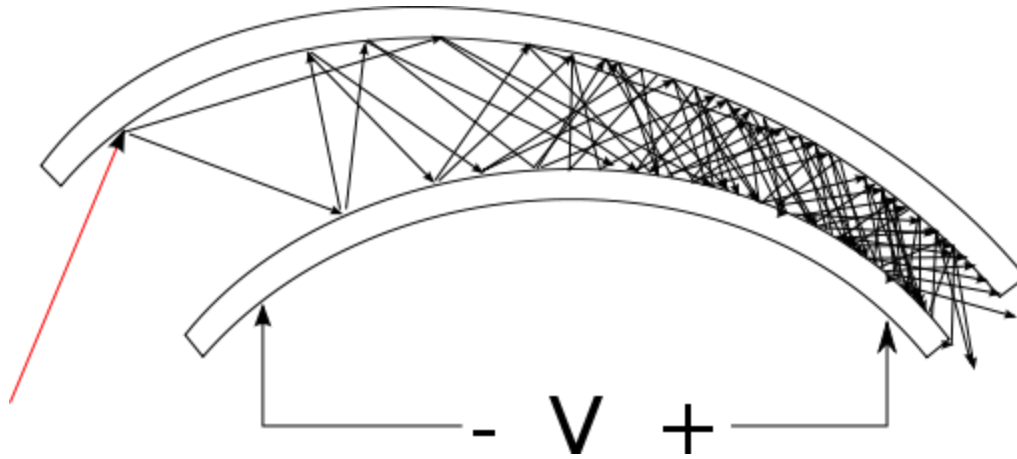
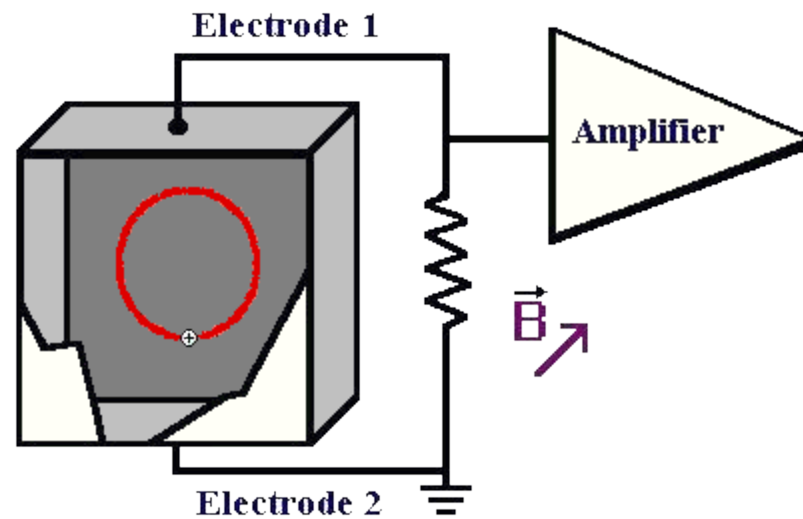
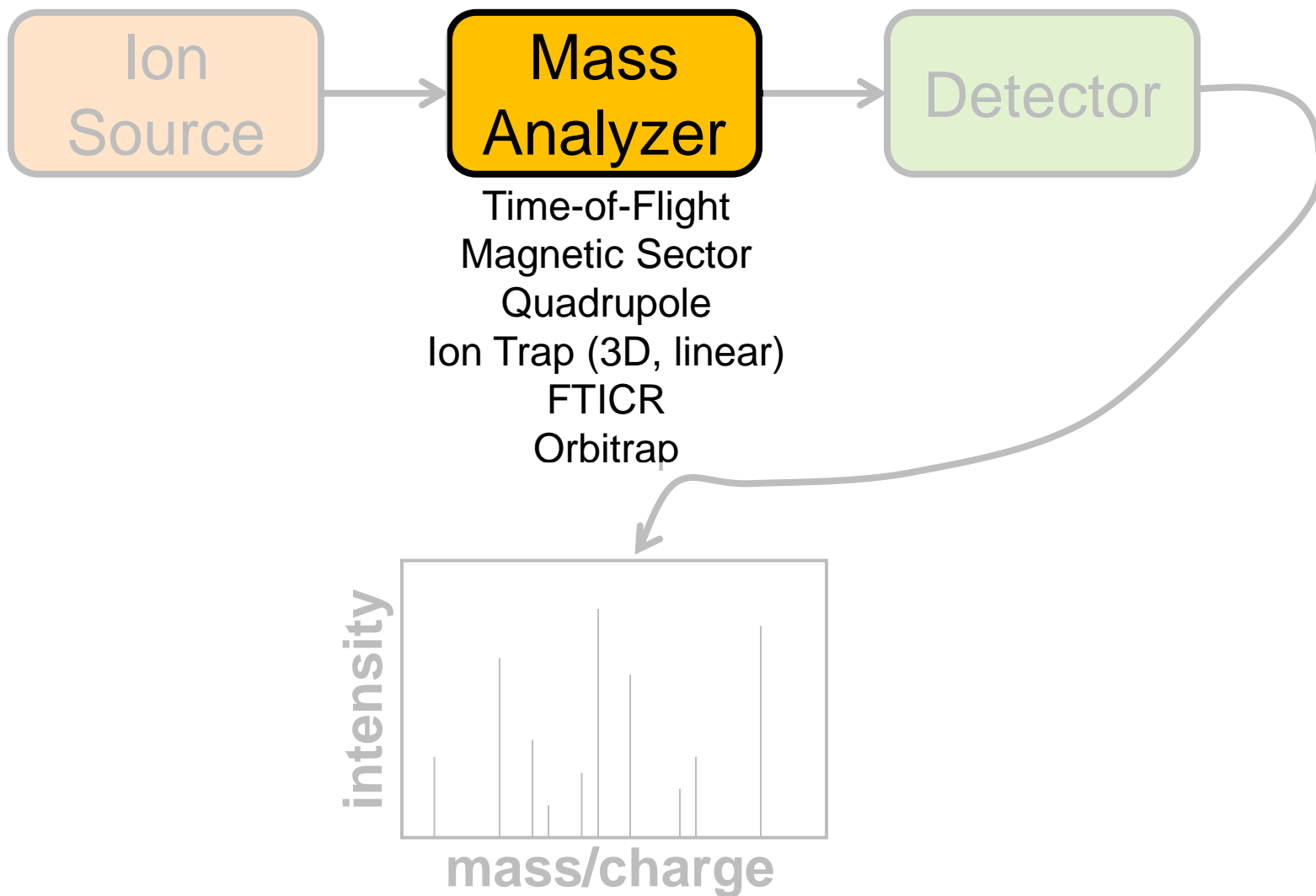


Image Current Detector

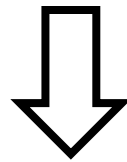


Mass Analyzers



Mass Spectrometry (MS)

$$\vec{F} = m\vec{a} = m \frac{d\vec{v}}{dt} = z(\vec{E} + \vec{v} \times \vec{B})$$

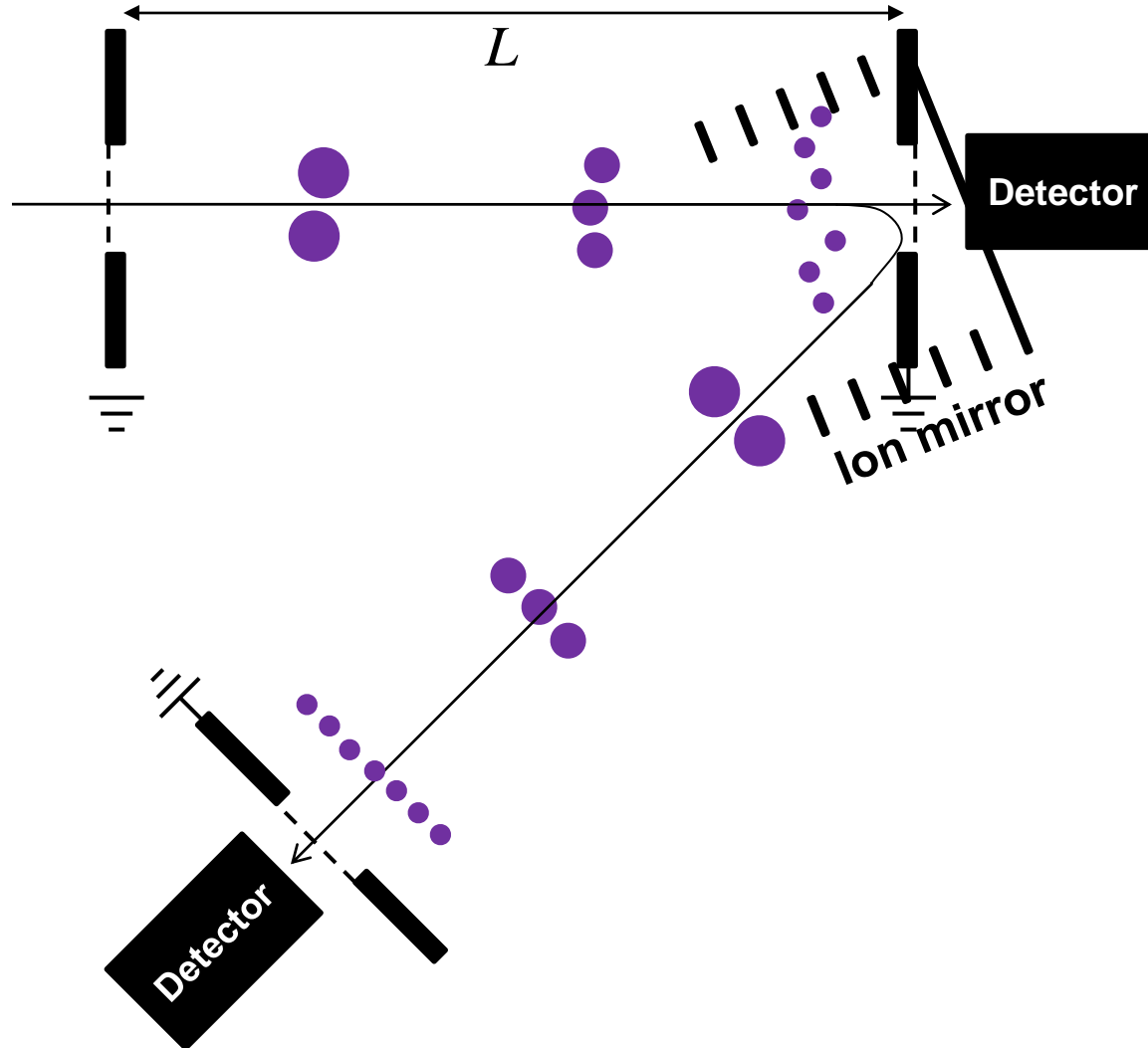


$$\boxed{\frac{m}{z}} \frac{d\vec{v}}{dt} = \vec{E} + \vec{v} \times \vec{B}$$

Time-of-Flight Mass Spectrometry

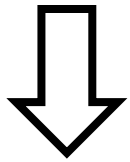


Time-of-Flight



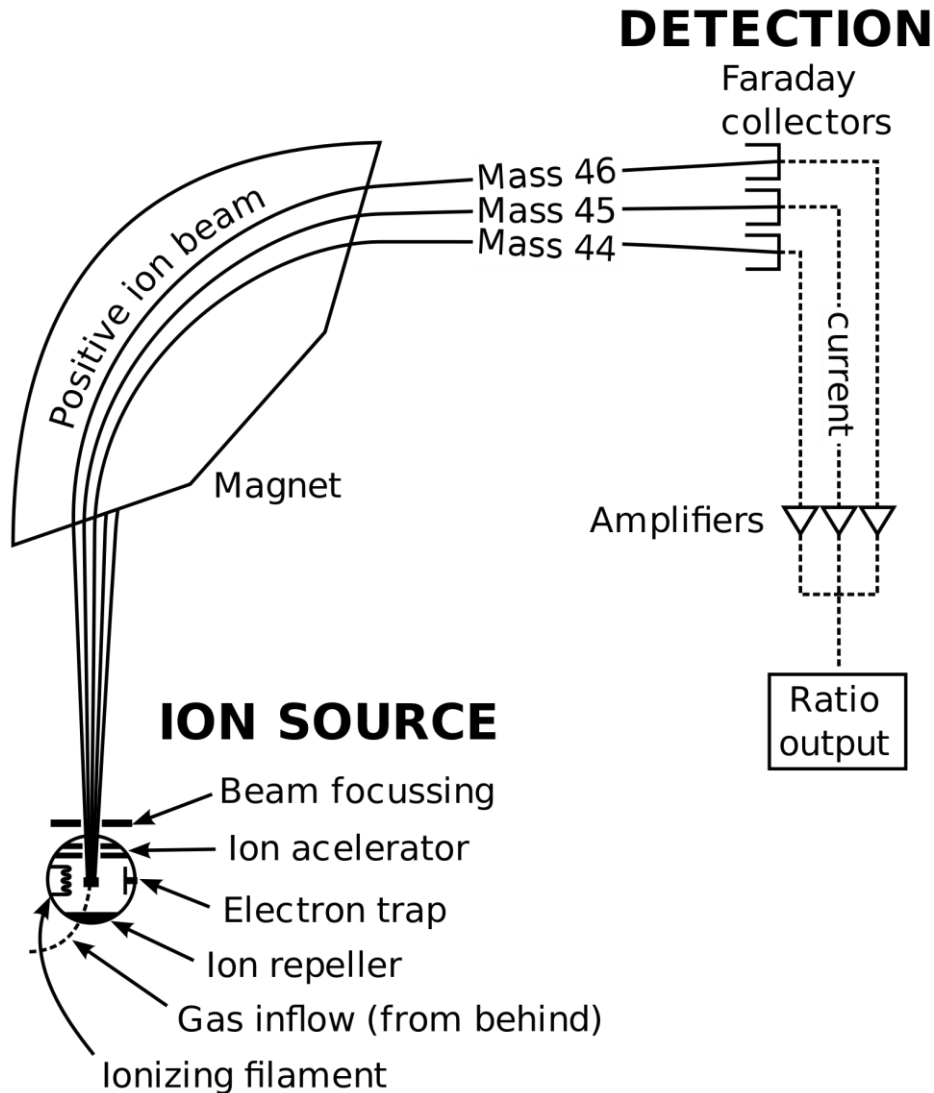
$$zV = \frac{mv^2}{2}$$

$$L = vt$$



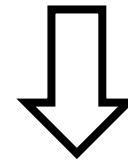
$$t = \frac{L}{\sqrt{2V}} \sqrt{\frac{m}{z}}$$

Magnetic Sector



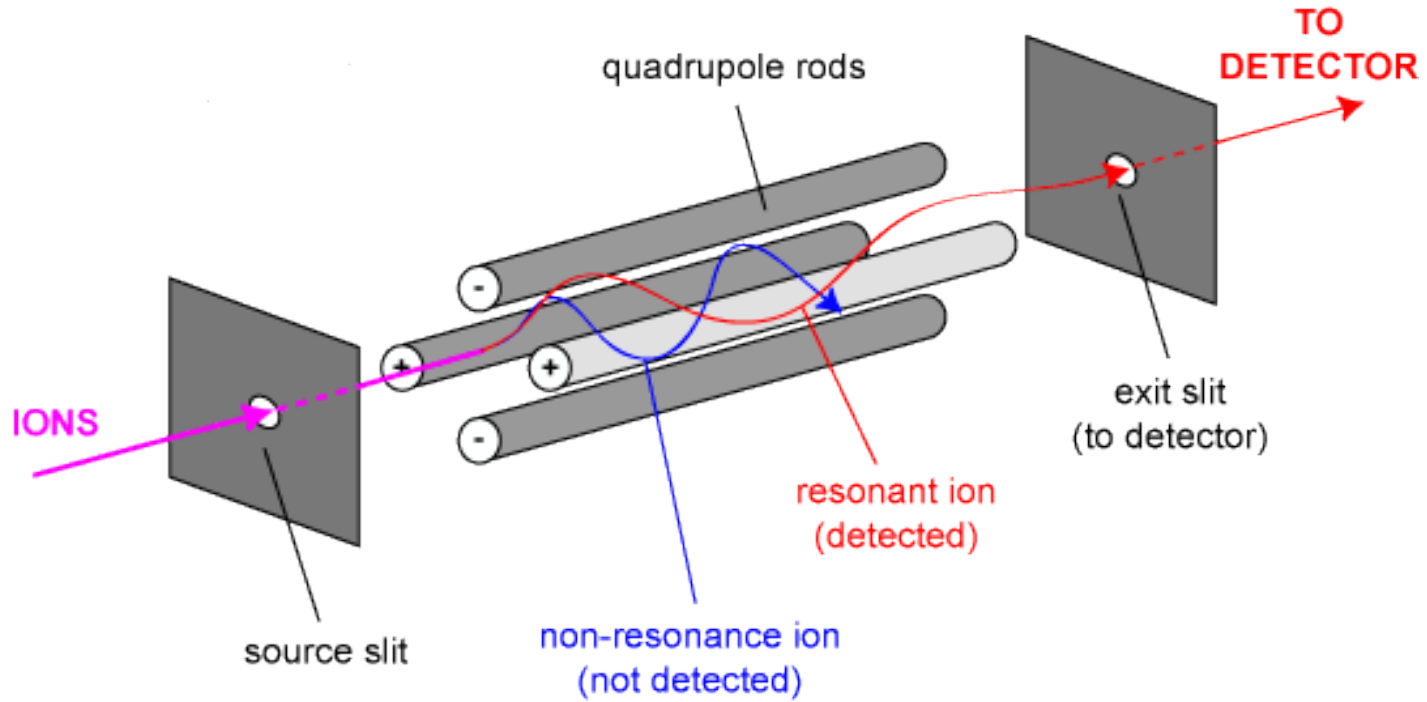
$$\overline{F} = \frac{mv^2}{R} = zvB$$

$$zV = \frac{mv^2}{2}$$



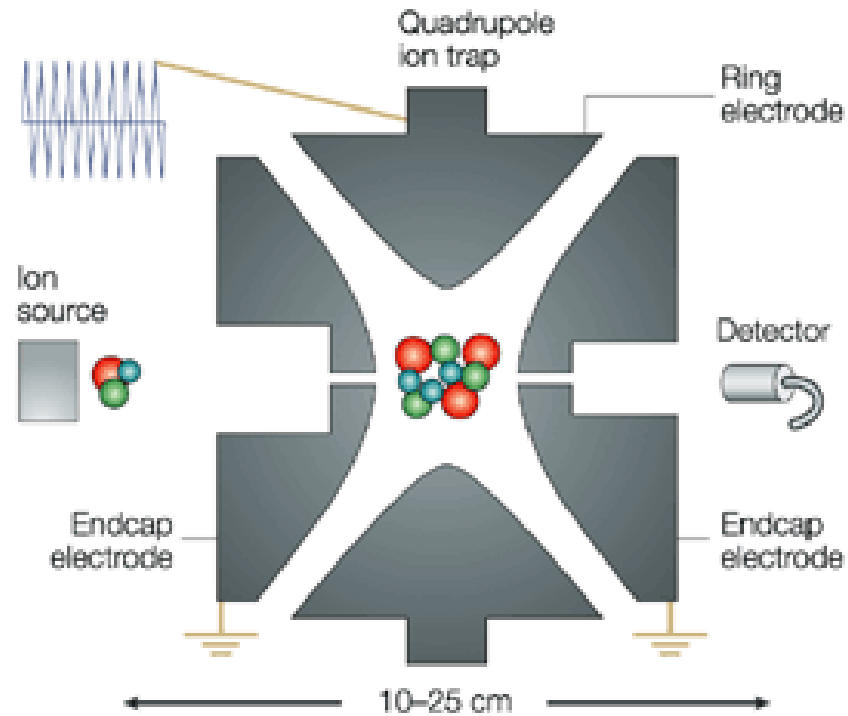
$$R = \sqrt{\frac{m}{z}} \sqrt{\frac{2V}{B}}$$

Quadrupole Mass Filter



$$\begin{array}{l} -U - V \cos(\omega t) \\ U + V \cos(\omega t) \end{array} \begin{array}{l} \uparrow y \\ \rightarrow x \end{array}$$

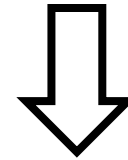
Ion Trap



Fourier transform ion cyclotron resonance



$$\bar{F} = \frac{mv^2}{R} = zvB$$



$$\boxed{\frac{m}{z}} = \frac{R}{v} B = \frac{B}{\omega}$$

Orbitrap

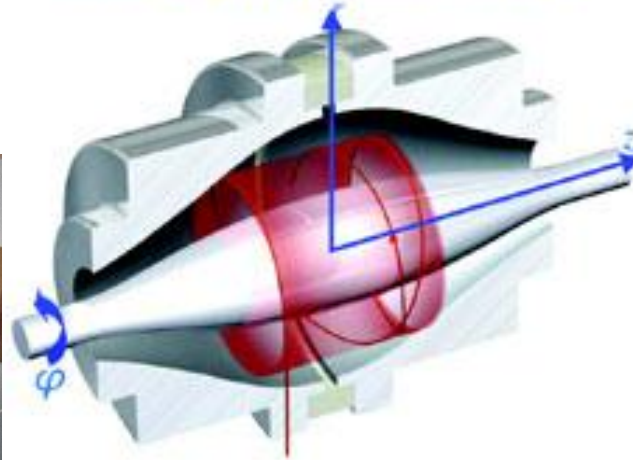
- Characteristic frequencies:

- Frequency of rotation ω_φ
- Frequency of radial oscillations ω_r
- Frequency of axial oscillations ω_z

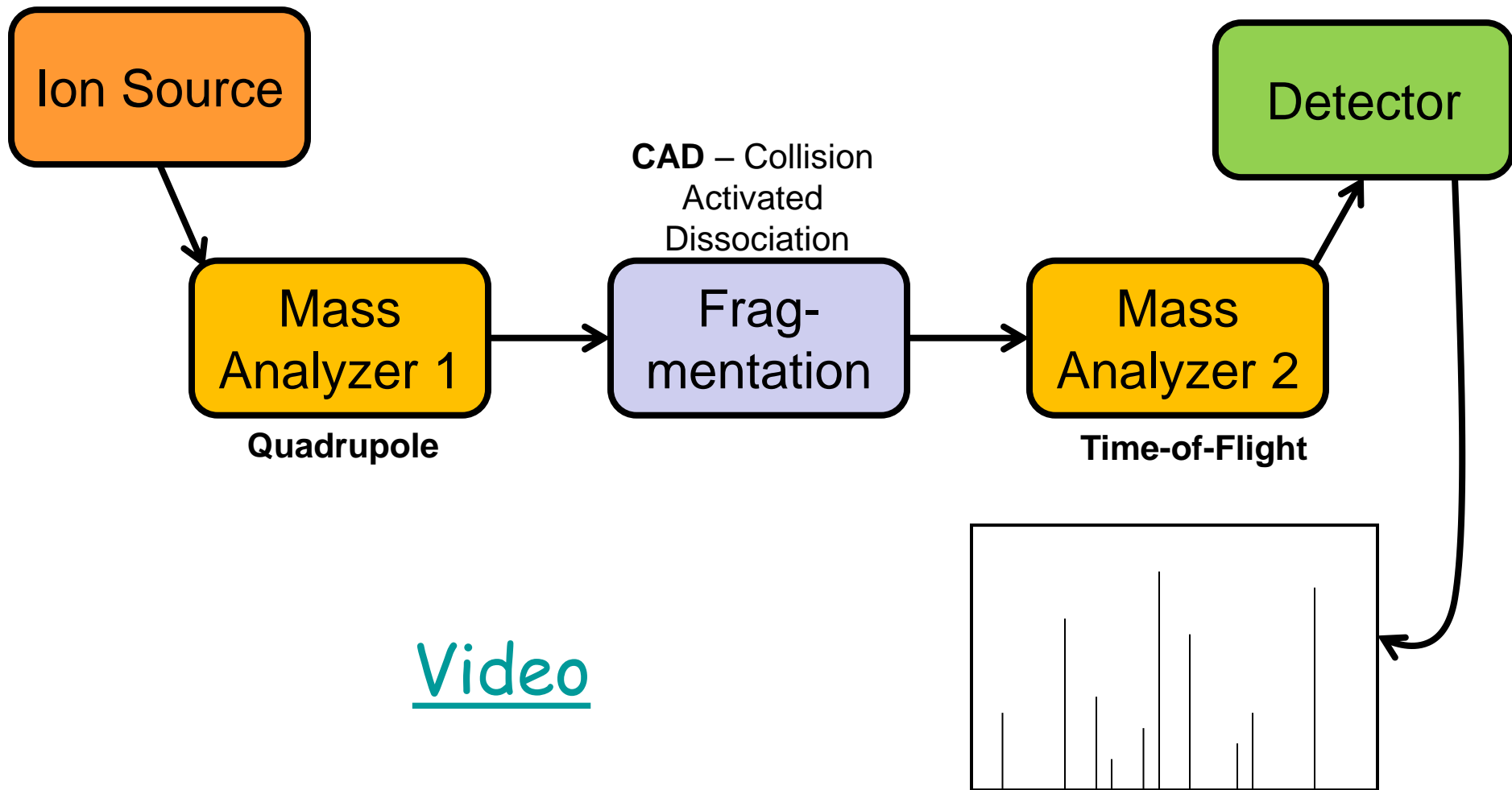
$$\omega_\varphi = \frac{\omega_z}{\sqrt{2}} \sqrt{\left(\frac{R_m}{R}\right)^2 - 1}$$

$$\omega_r = \omega_z \sqrt{\left(\frac{R_m}{R}\right)^2 - 2}$$

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

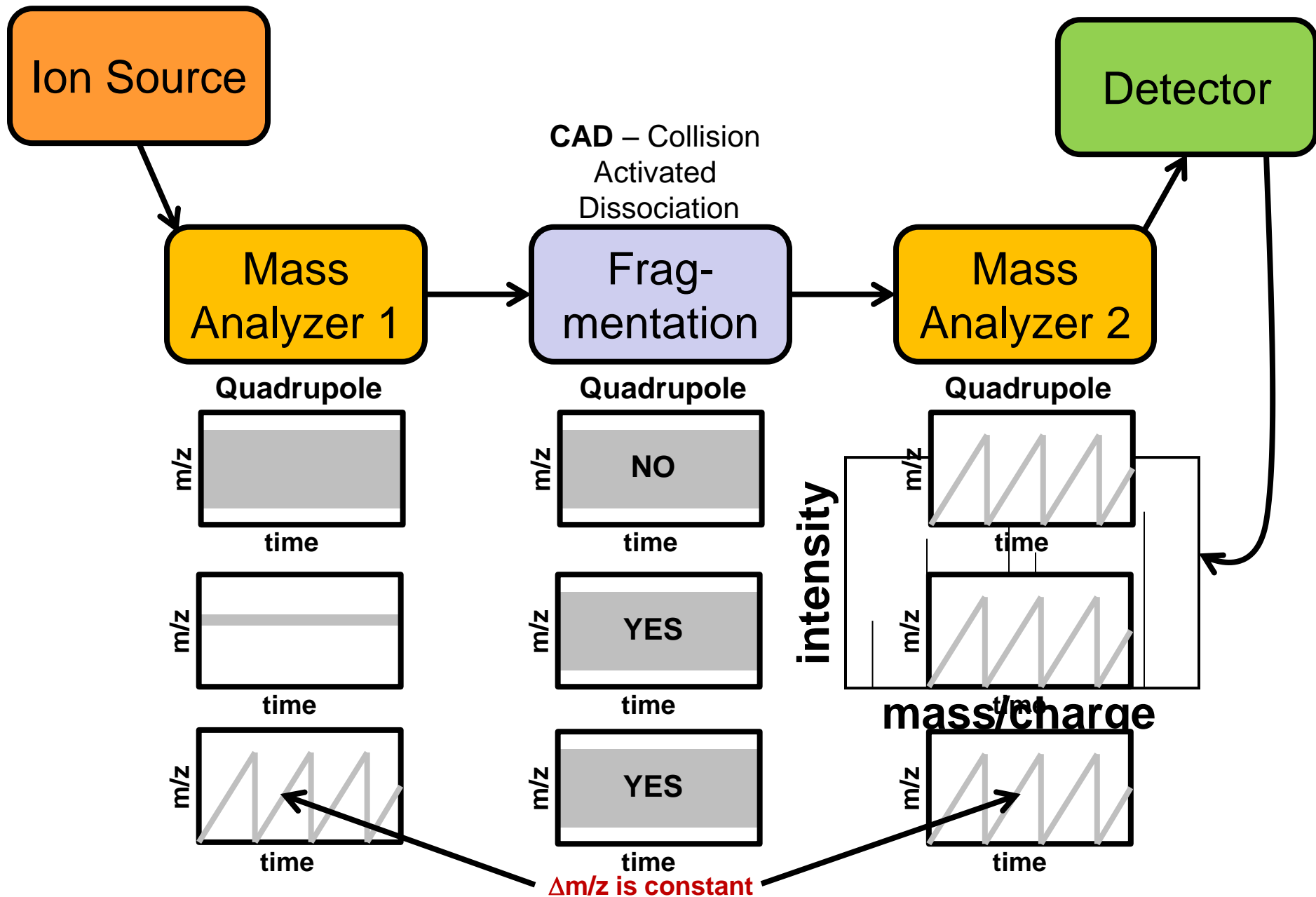


Quadrupole Time-of-Flight Mass Spectrometer

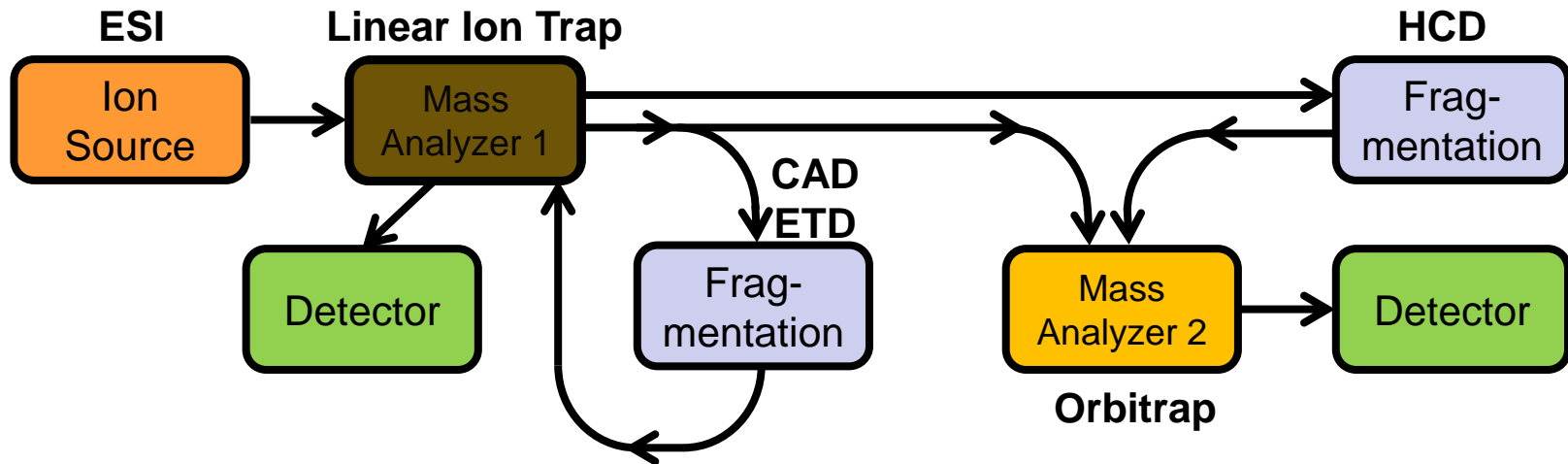


[Video](#)

Triple Quadrupole



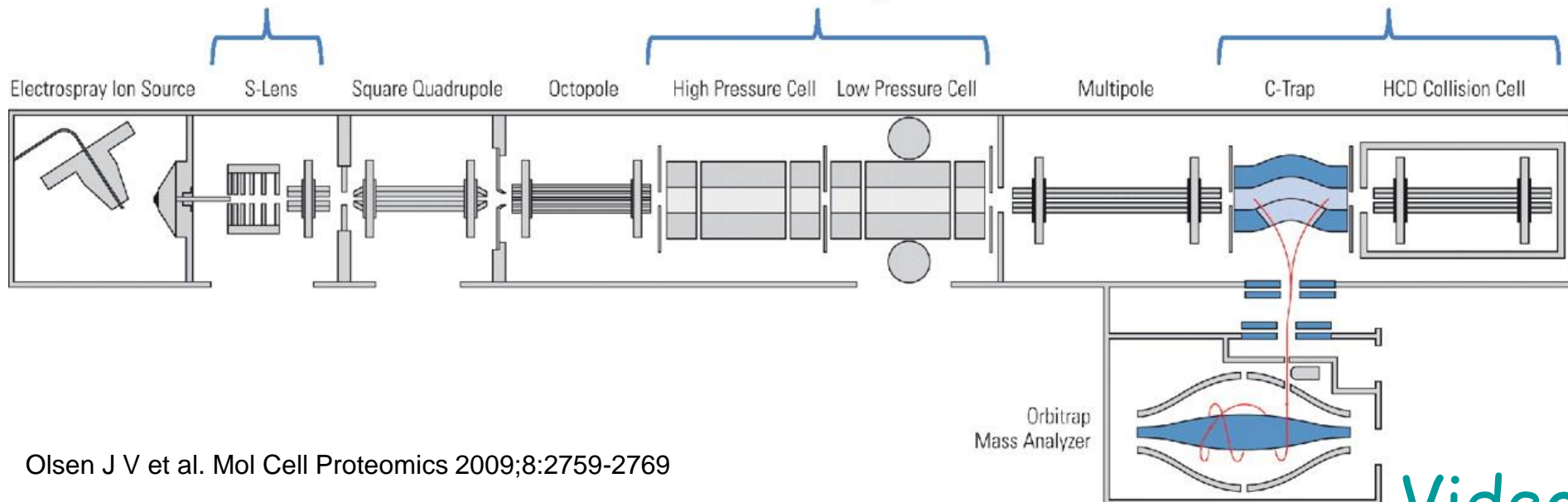
Linear Ion Trap / Orbitrap



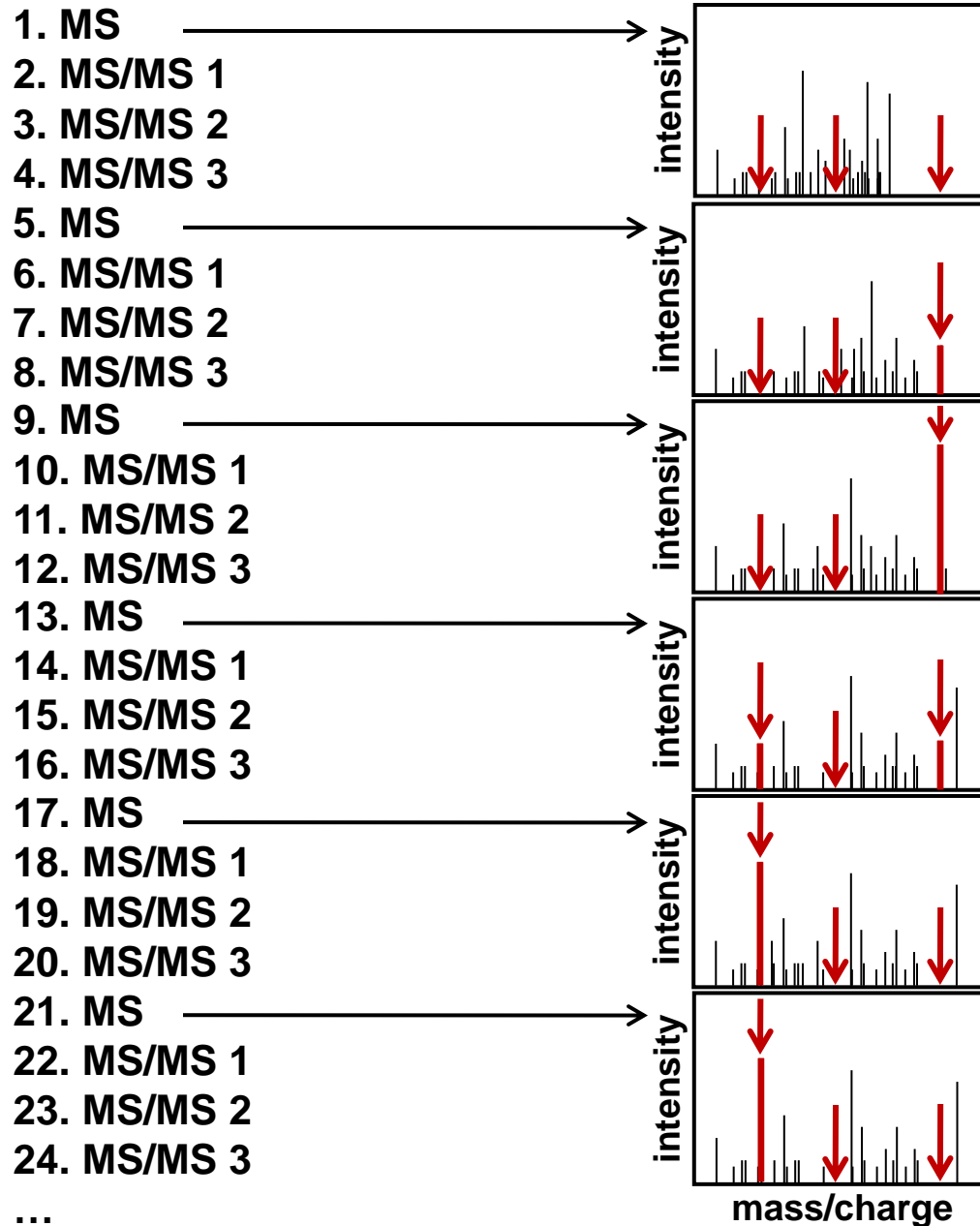
A. Stacked Ring Ion Guide

B. Dual linear ion trap

Combo C-trap/
C. HCD collision cell

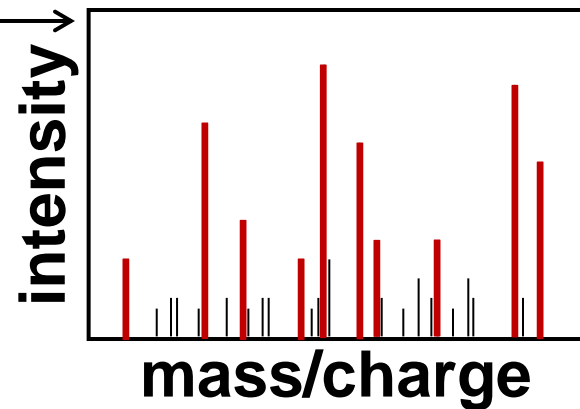


Data Independent Acquisition



Data Dependent Acquisition

1. MS



12. MS

13. MS/MS 1

14. MS/MS 2

15. MS/MS 3

16. MS/MS 4

17. MS/MS 5

18. MS/MS 6

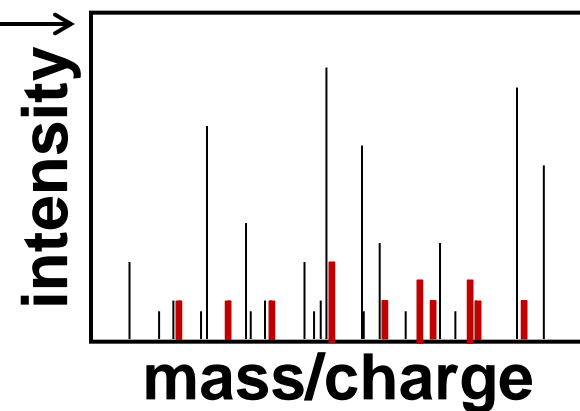
19. MS/MS 7

20. MS/MS 8

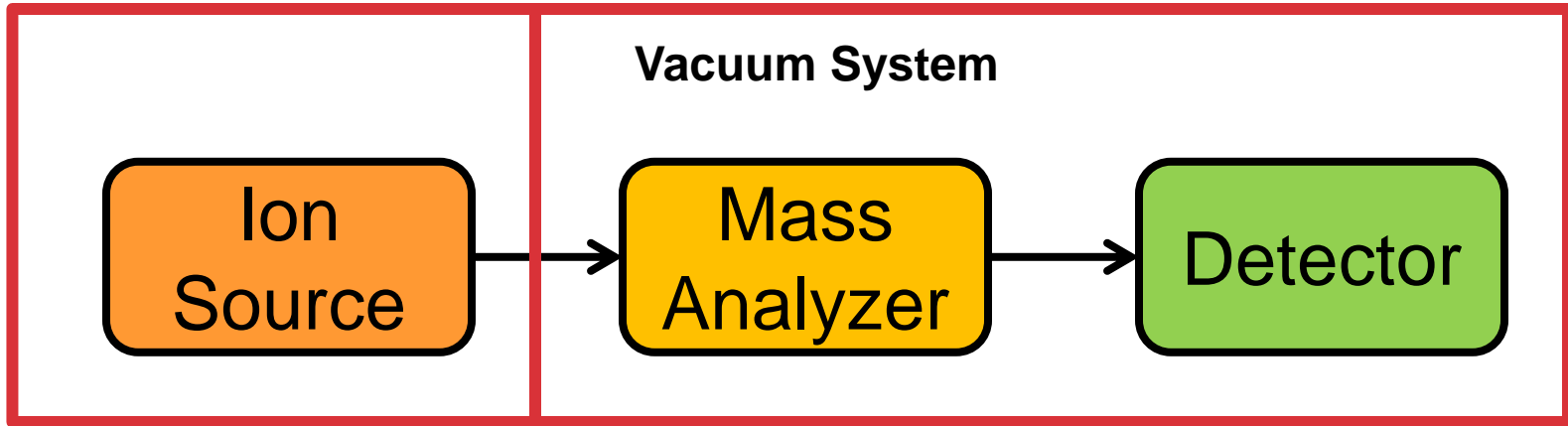
21. MS/MS 9

22. MS/MS 10

...



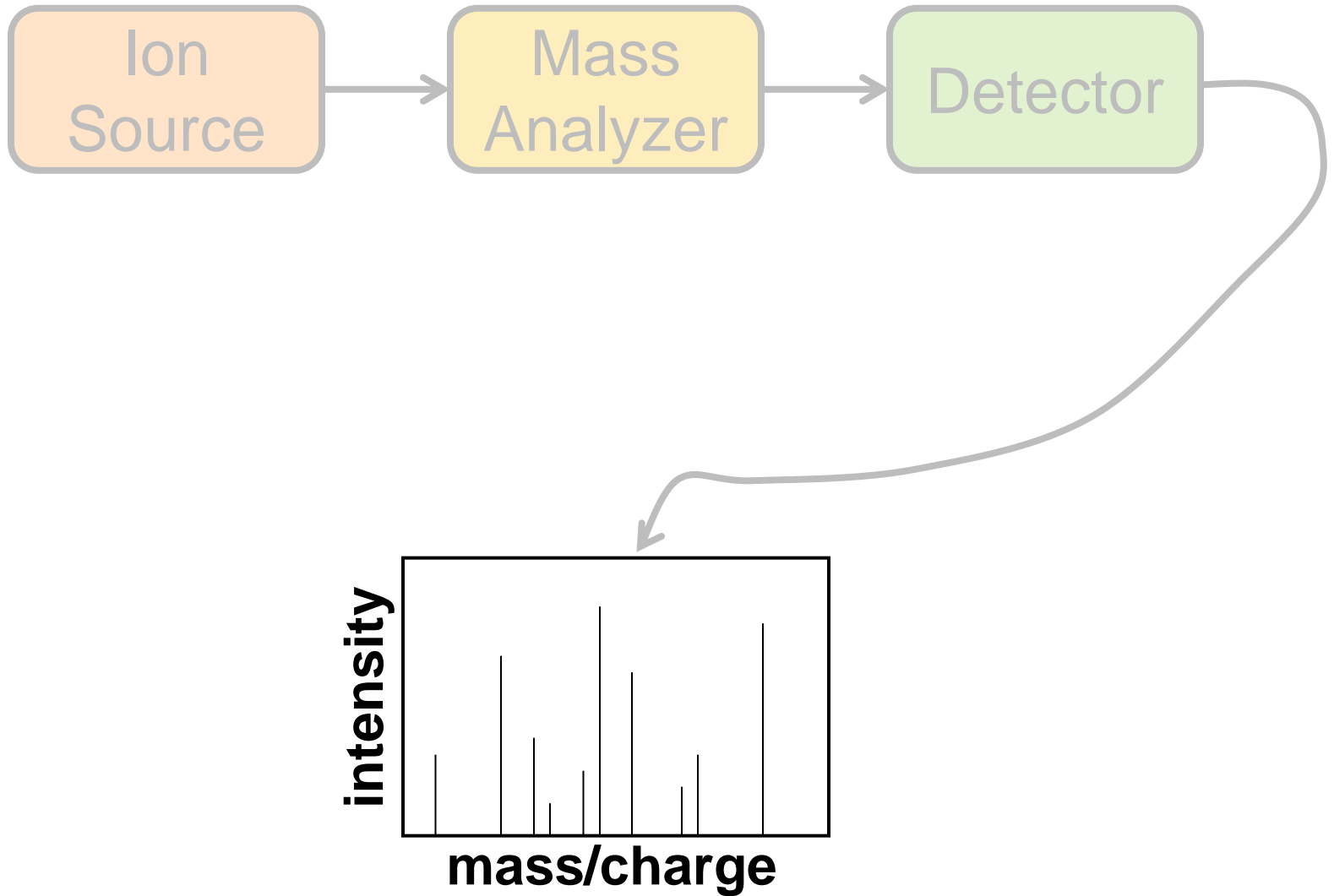
Vacuum System



Atmosphere



Mass Spectrometry Data



Mass Spectrometry Data

Dimensions:

Time

Peptide m/z

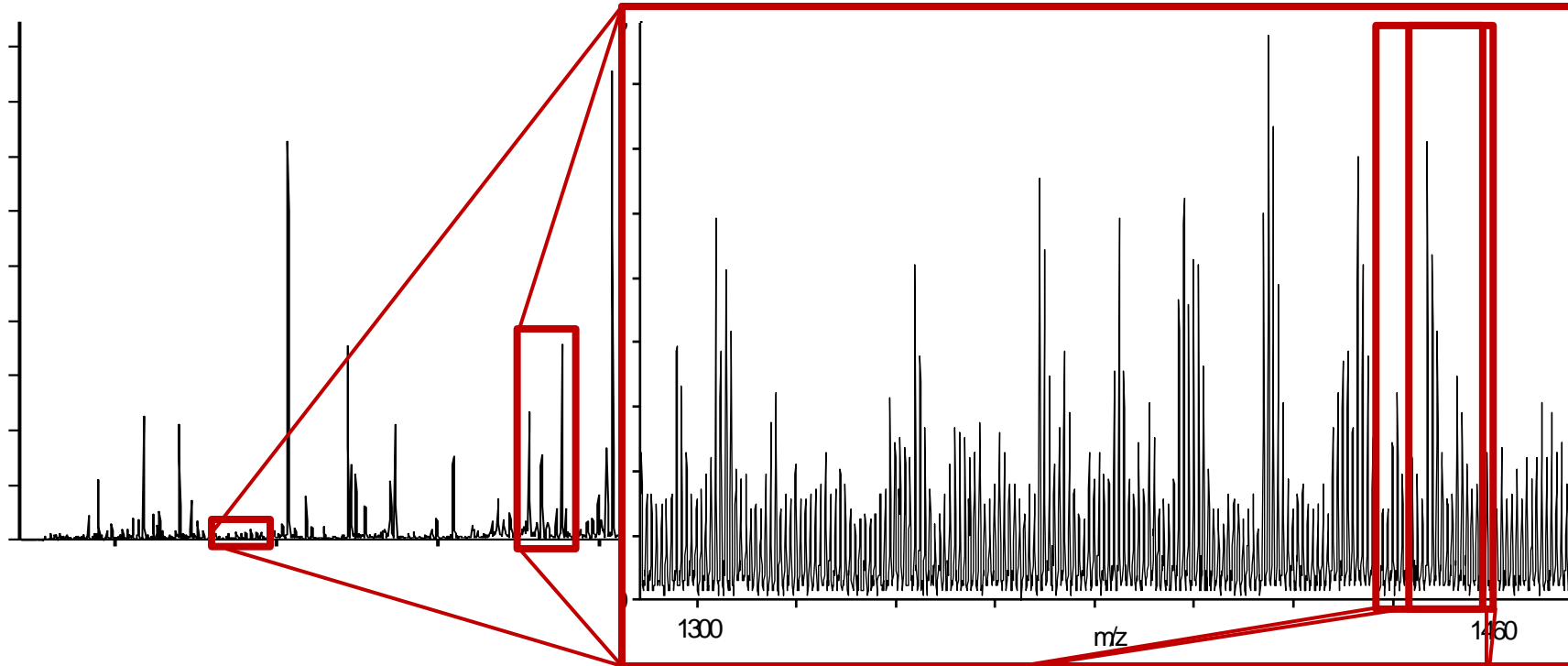
Peptide Intensity

Peptide fragment m/z

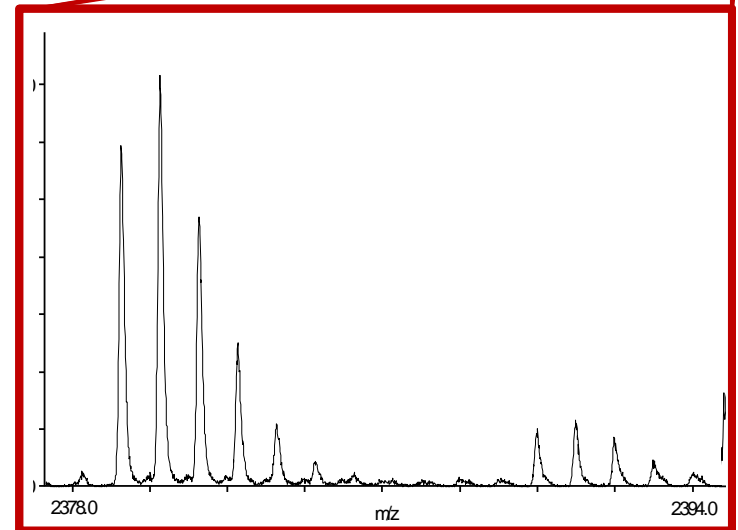
Peptide fragment intensity

...

Example data - MALDI-TOF

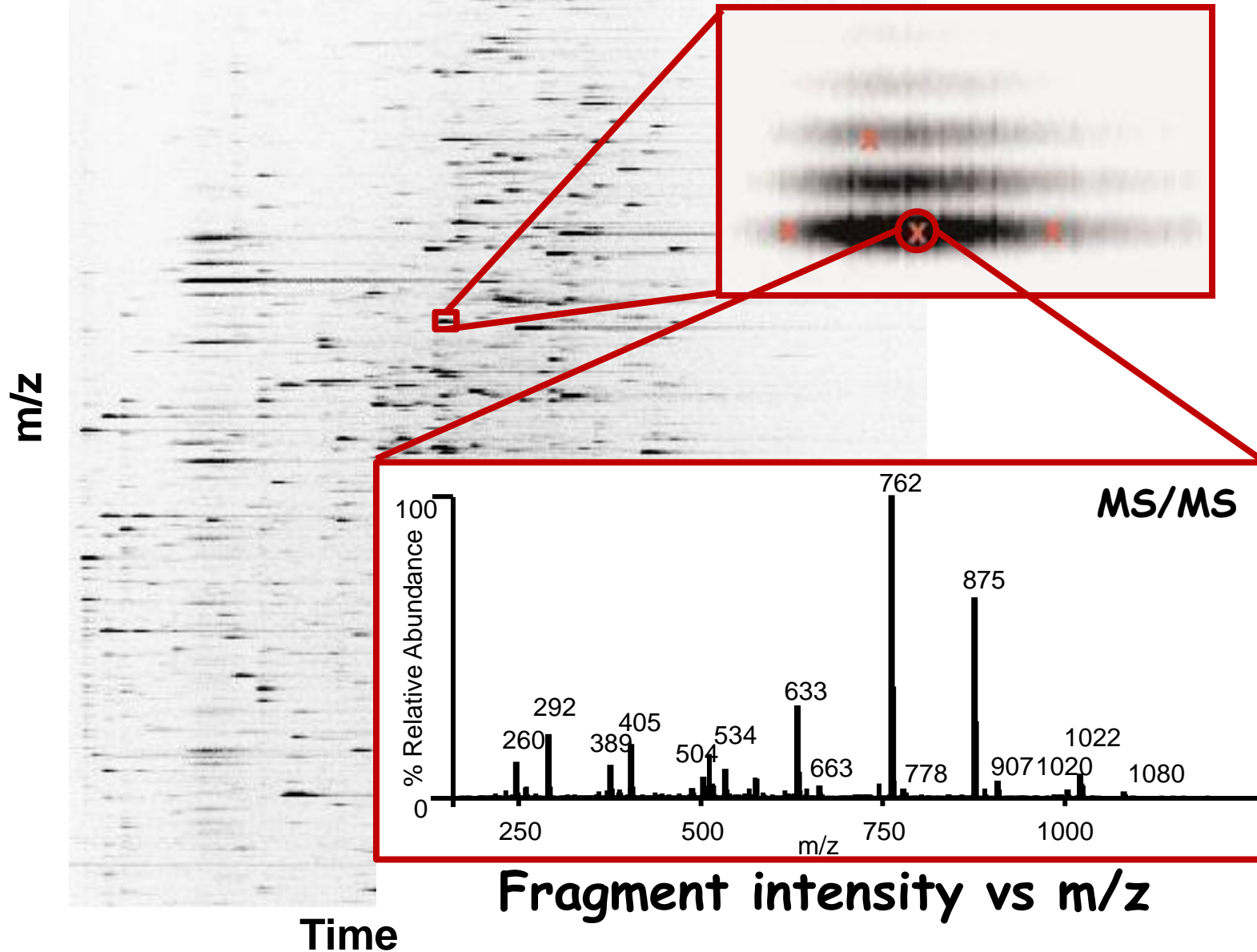


Peptide intensity vs m/z




Example data - ESI-LC-MS/MS

Peptide intensity vs m/z vs time



Slice - Scalable Data Sharing for Remote Mass Informatics

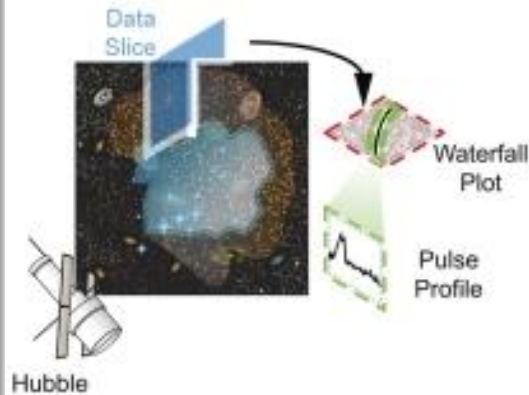


YIVSGTPTFPVPLIK => 849.480 2

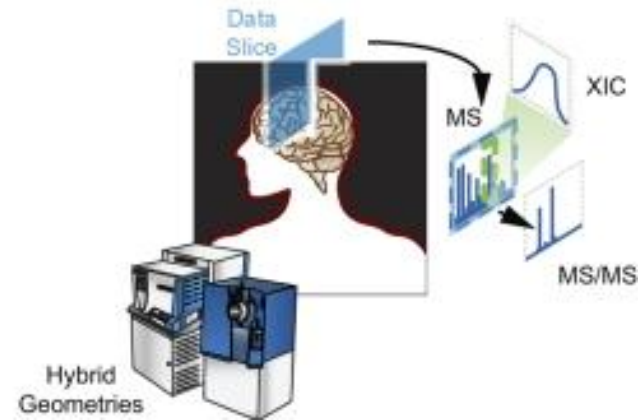
Filename	Time	Intensity	Preview	MS2
Roche_human_CSF_017	71.689	2389918		✓
Roche_human_CSF_021	76.772	1242552		✓
Roche_human_CSF_018	72.168	1003575		✓
Roche_human_CSF_046	40.513	953971		✓
Roche_human_CSF_014	71.517	932062		✓
Roche_human_CSF_022	72.896	757225		✓
Roche_human_CSF_013	77.03	439764		✓
Roche_human_CSF_019	74.551	397208		✓
Roche_human_heart_191	45.874	230045		
Roche_human_heart_023	35.45	208049		

Developed by Manor Askenazi
slice.ionomix.com

Mapping Celestial Features



Mapping Human Proteins



Most mass spectrometry data is acquired in discovery mode, meaning that the data is amenable to open-ended analysis as our understanding of the target biochemistry increases. In this sense, mass spectrometry based discovery work is more akin to an astronomical survey, where the full list of object-types being imaged has not yet been fully elucidated, as opposed to e.g. micro-array work, where the list of probes spotted onto the slide is finite and well understood.

Example Mass Spectrometry Data

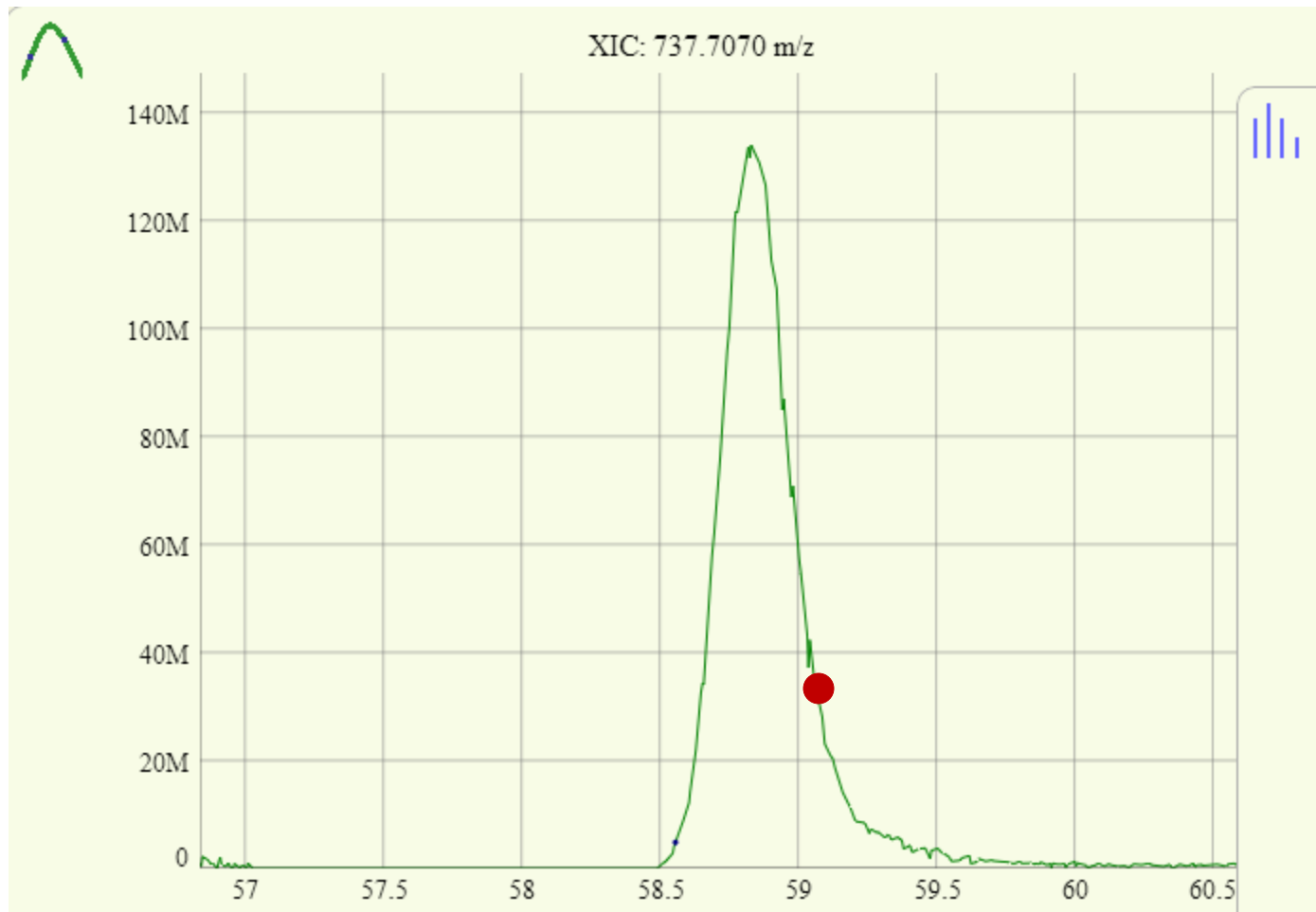


The image shows the 'Slice' software interface. At the top, the word 'Slice' is written in large, stylized green letters. To the right of the text is a 3D illustration of a whole yellow lemon and two slices, one showing the internal segments. Below the title, there is a search bar containing the peptide sequence 'LGEHNIDVLEGNEQFINAAK'. To the right of the search bar is an arrow pointing to a box containing the m/z value '737.707', followed by a small box with the number '3' and up/down arrows. Further right is a button with a lemon slice icon and the text 'Slice!'. Below these controls is a table with five columns: 'Filename', 'Time', 'Intensity', 'Preview', and 'MS2'. The table contains three rows of data, each with a small blue peak graph in the 'Preview' column and a green checkmark in the 'MS2' column.

Filename	Time	Intensity	Preview	MS2
101512_jrc_ecoli_yeast1	59.088	196495056		✓
101512_jrc_ecoli_yeast05	59.075	158554480		✓
101512_jrc_ecoli	58.831	133886480		✓

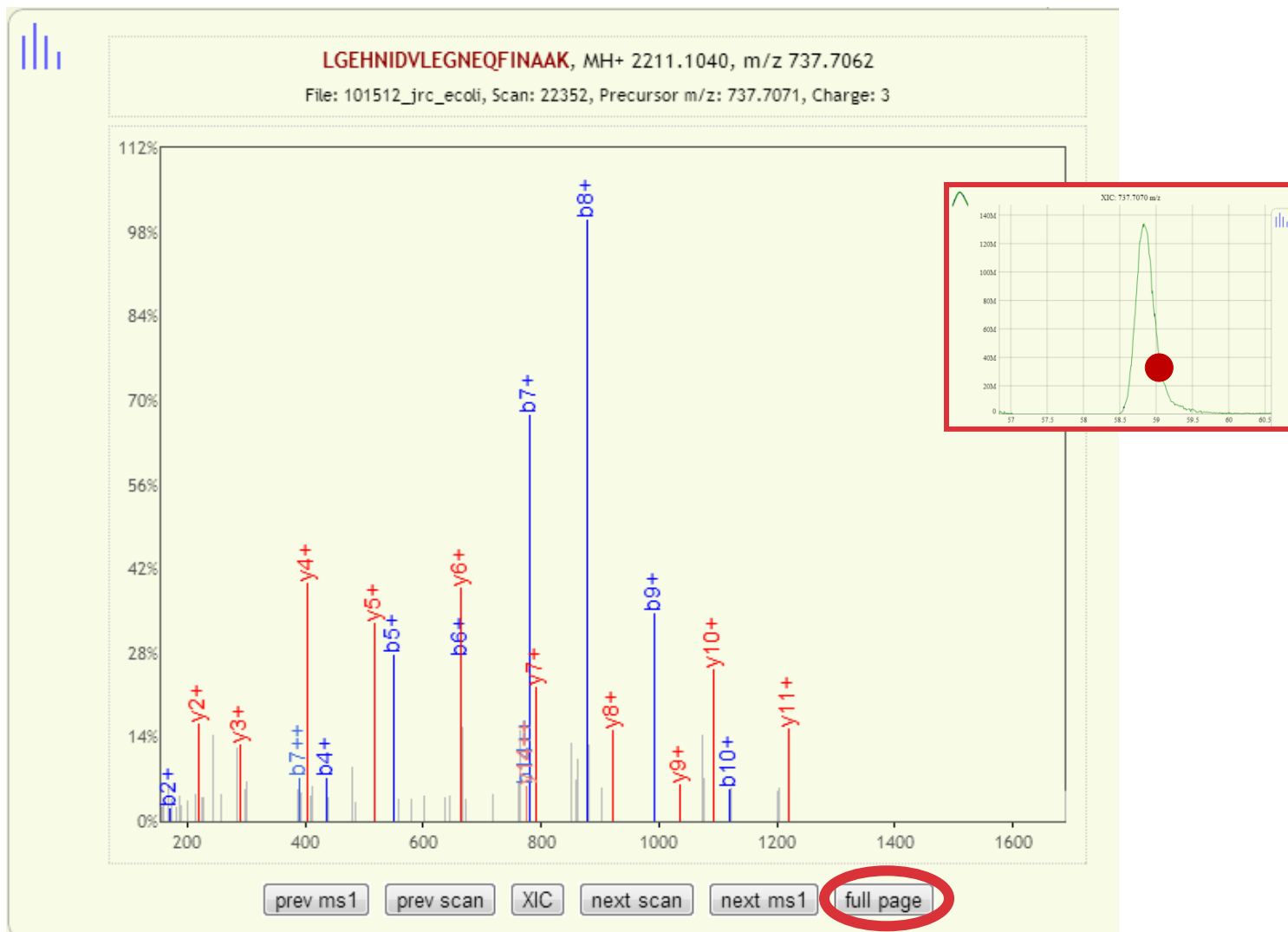
fenyolab.ionomix.com

Example Mass Spectrometry Data



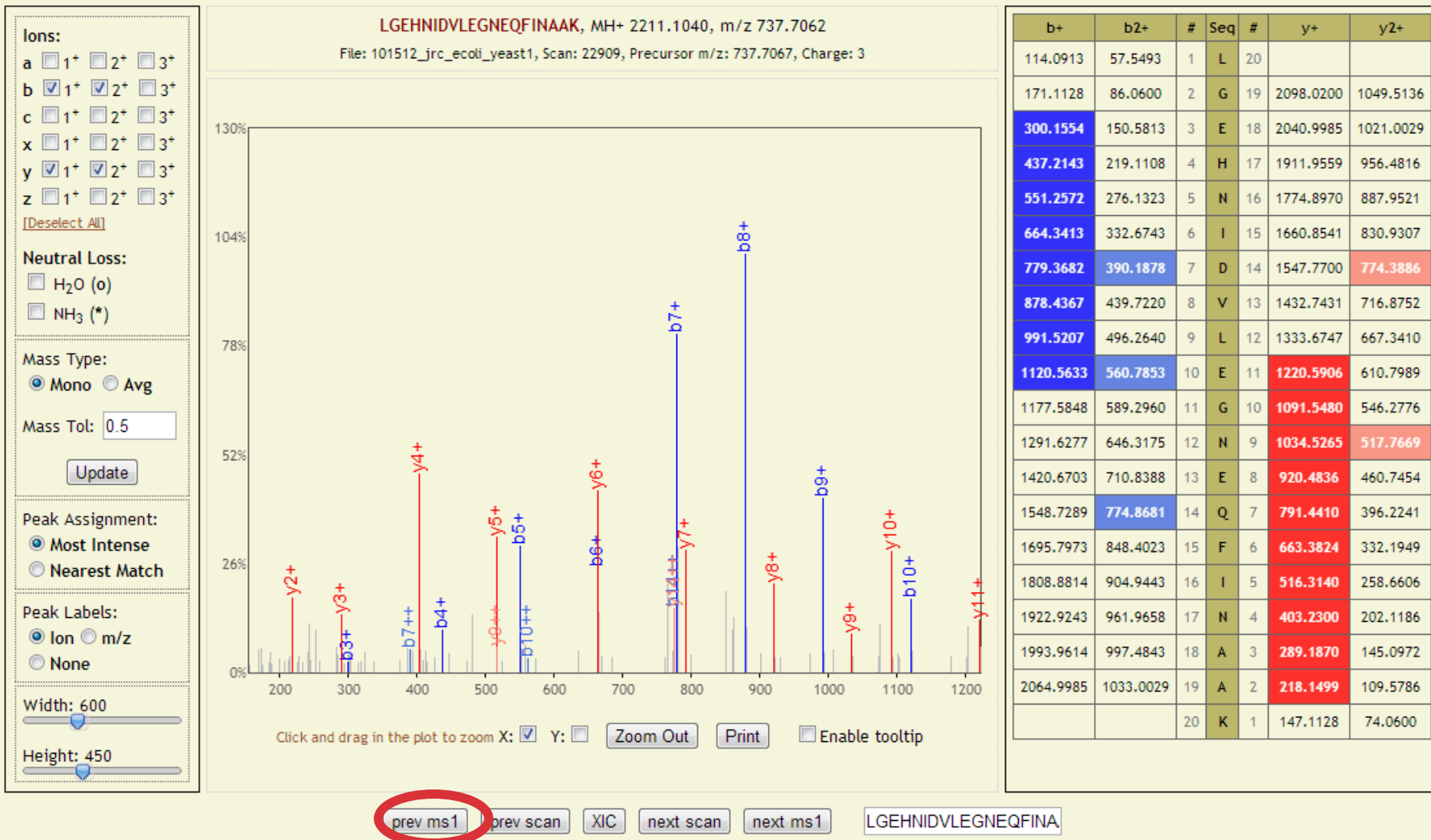
Peptide intensity vs time
For 737.707 m/z which corresponds to
3+ of LGEHNIDVLEGNEQFINAAK

Example Mass Spectrometry Data



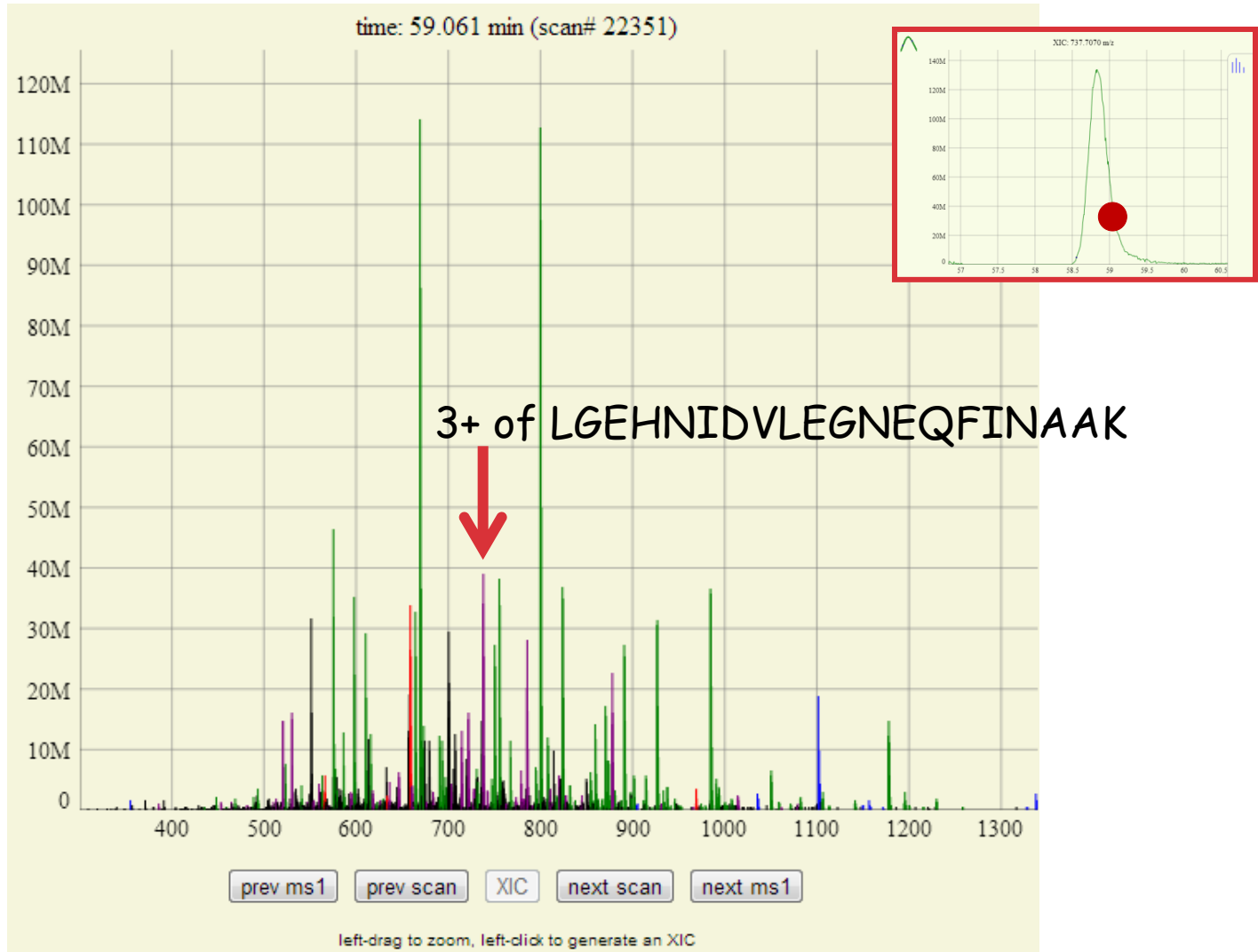
Fragment intensity vs m/z
For 3+ of LGEHNIDVLEGNEQFINAAK

Example Mass Spectrometry Data



Fragment intensity vs m/z
 For 3+ of LGEHNIDVLEGNEQFINAAK

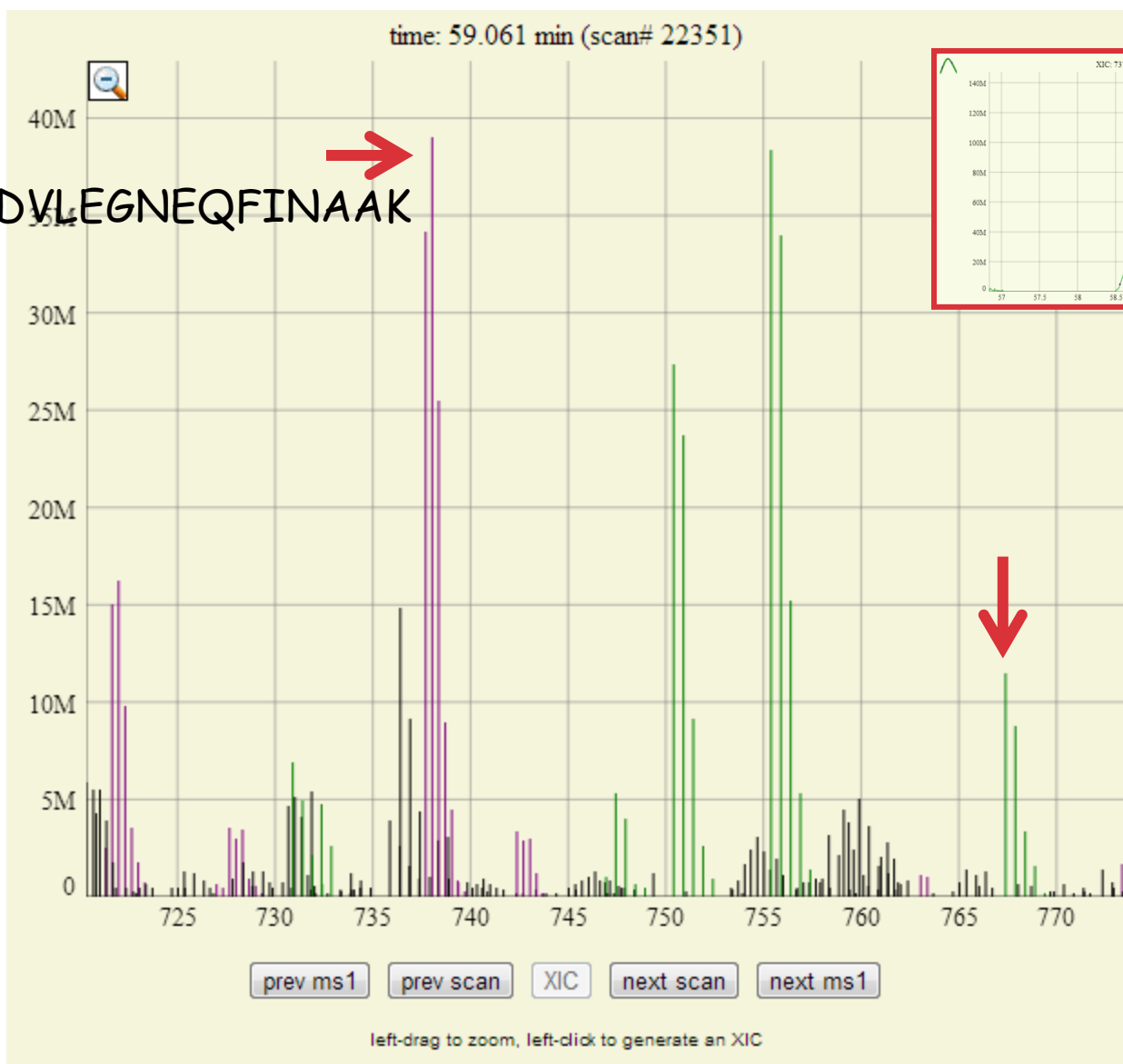
Example Mass Spectrometry Data



Peptide intensity vs m/z

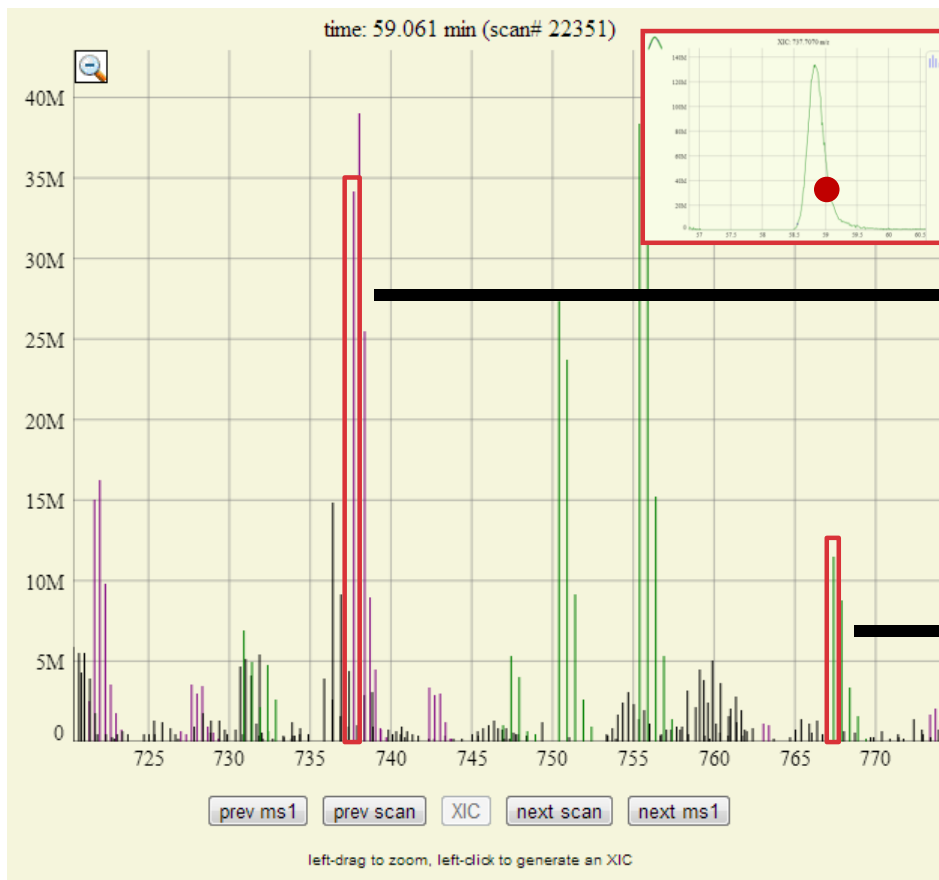
Example Mass Spectrometry Data

3+ of LGEHNIDVLEGNEQFINAAK

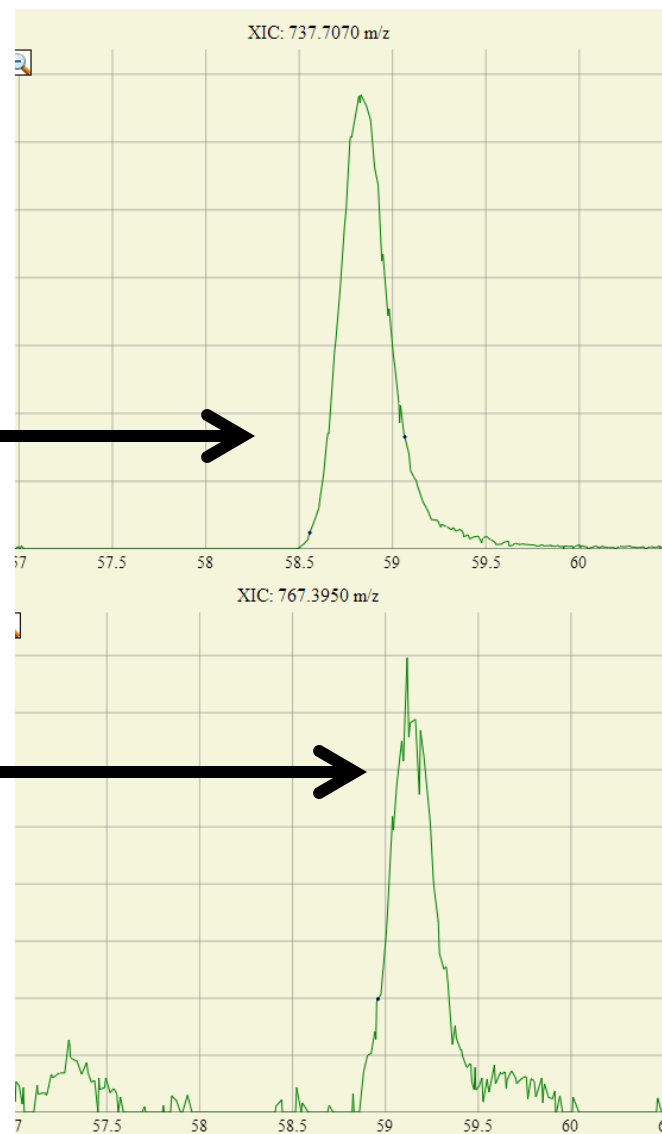


Peptide intensity vs m/z

Example Mass Spectrometry Data



Peptide intensity vs m/z



Peptide intensity vs time

Example Mass Spectrometry Data

ASTHTDSSAQTVSLEDYVSR 3+ in E. coli

DTTTIIDGVGEEAAIQGR 2+ in E. coli

ATGTSEMAPALVAAFVGGK 2+ in E. coli

FVPDTQAPLGIR 2+ in E. coli

Proteomics Informatics - Overview of Mass spectrometry (Week 2)

