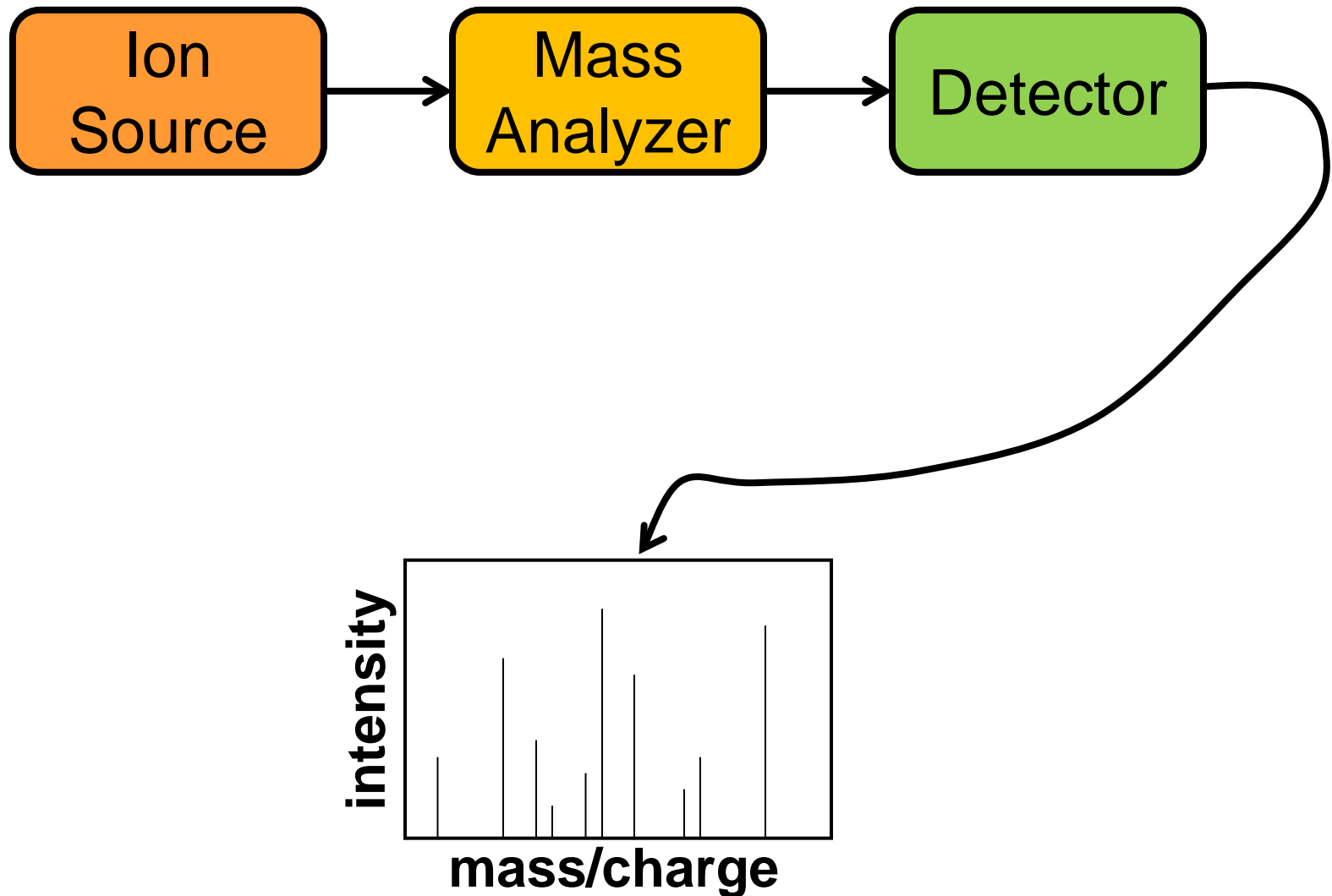
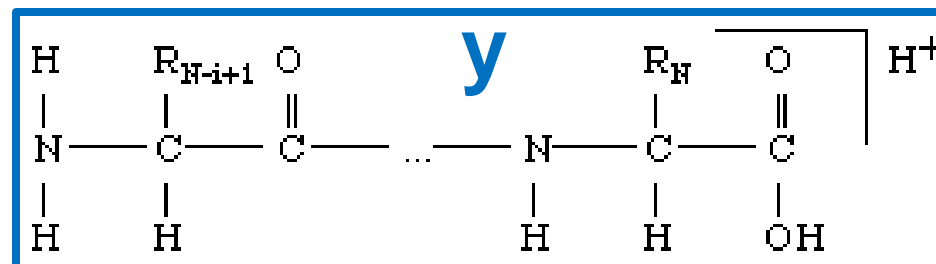
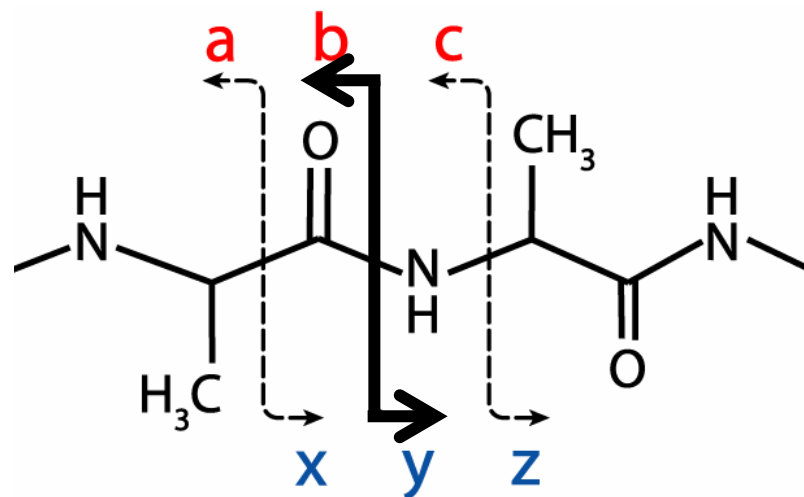
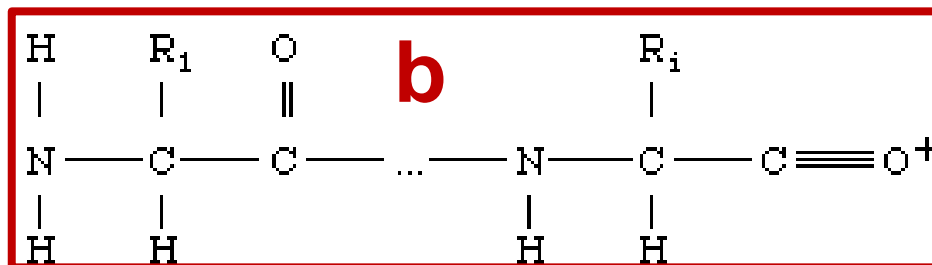


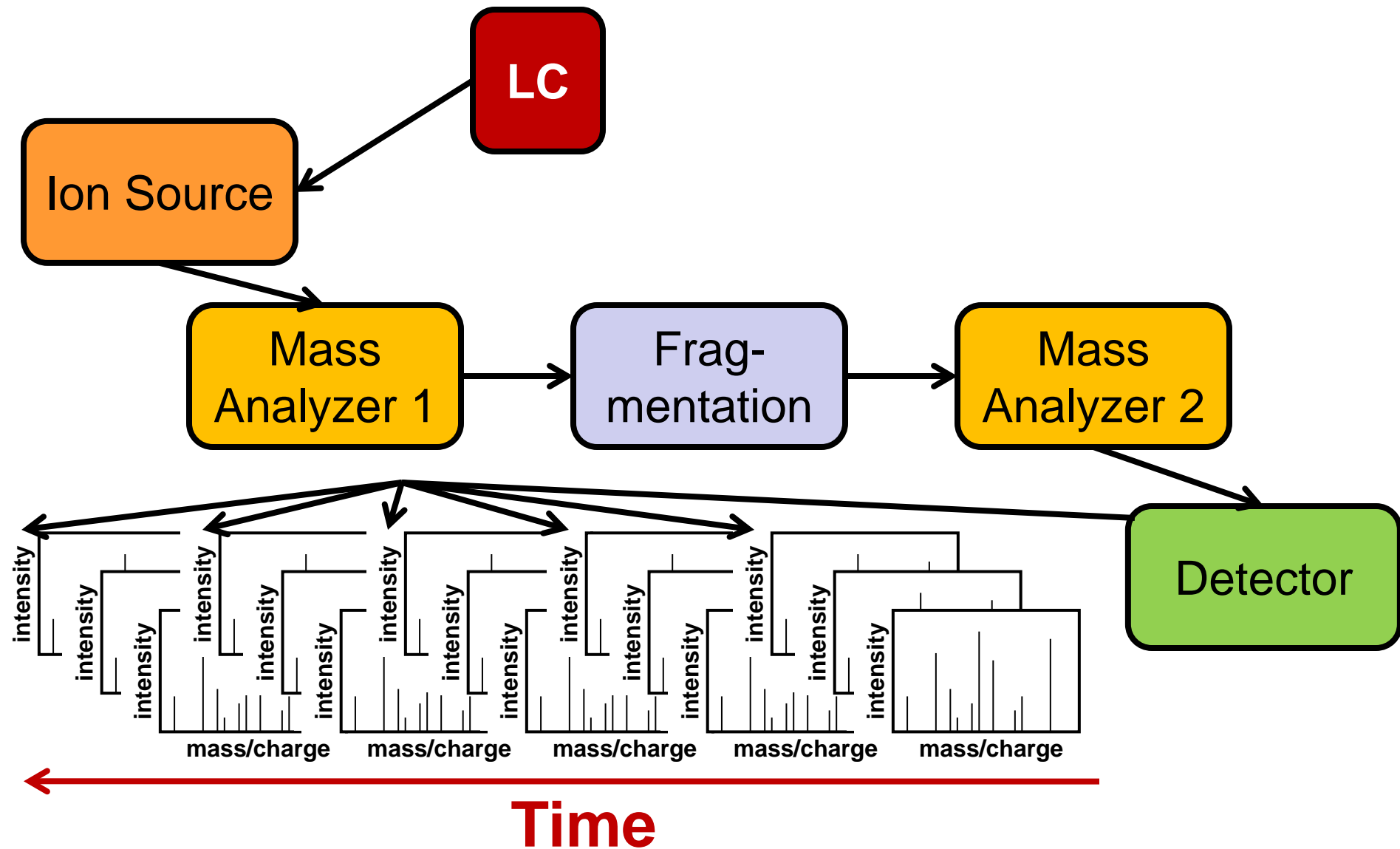
Proteomics Informatics - Overview of Mass spectrometry (Week 2)



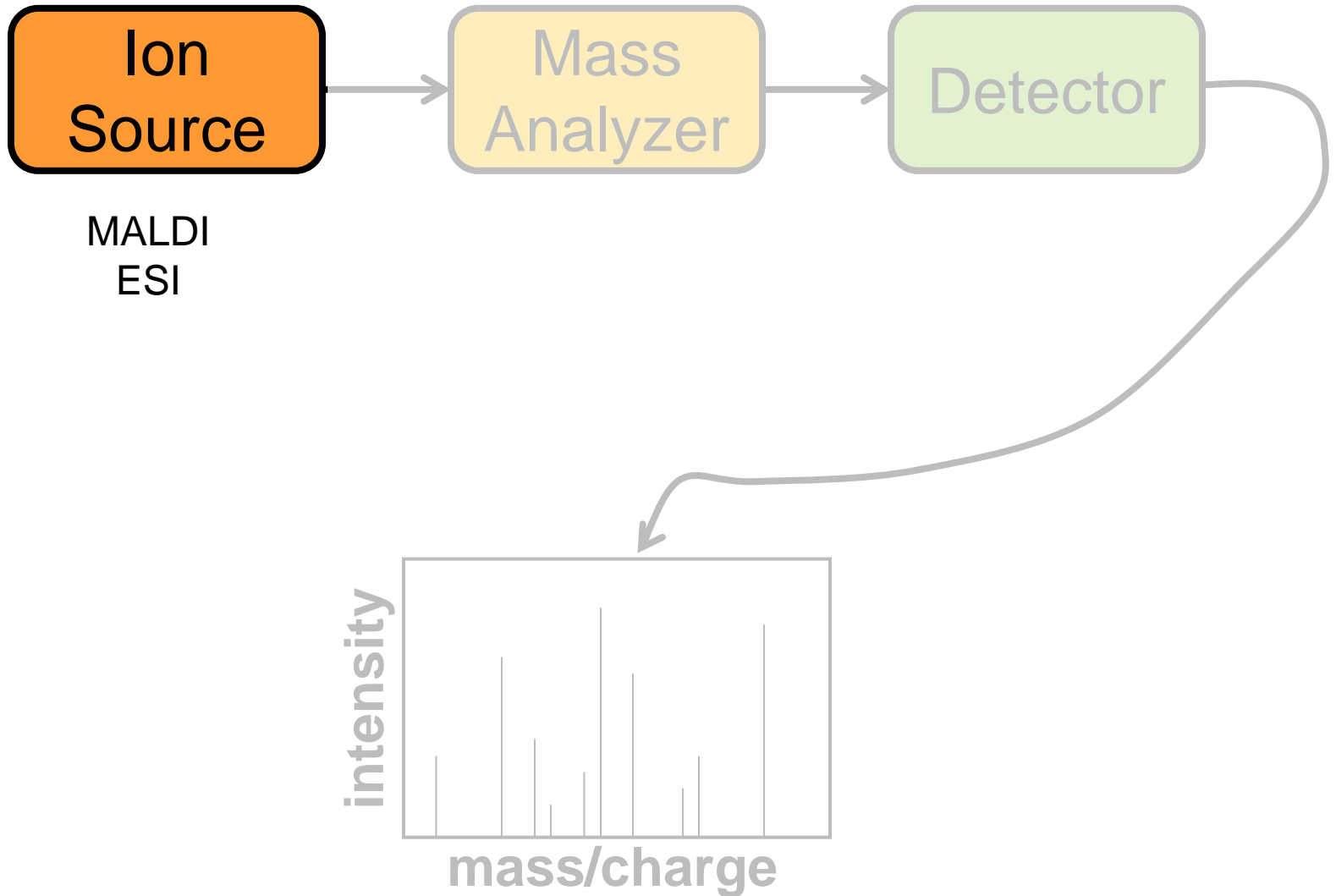
Peptide Fragmentation



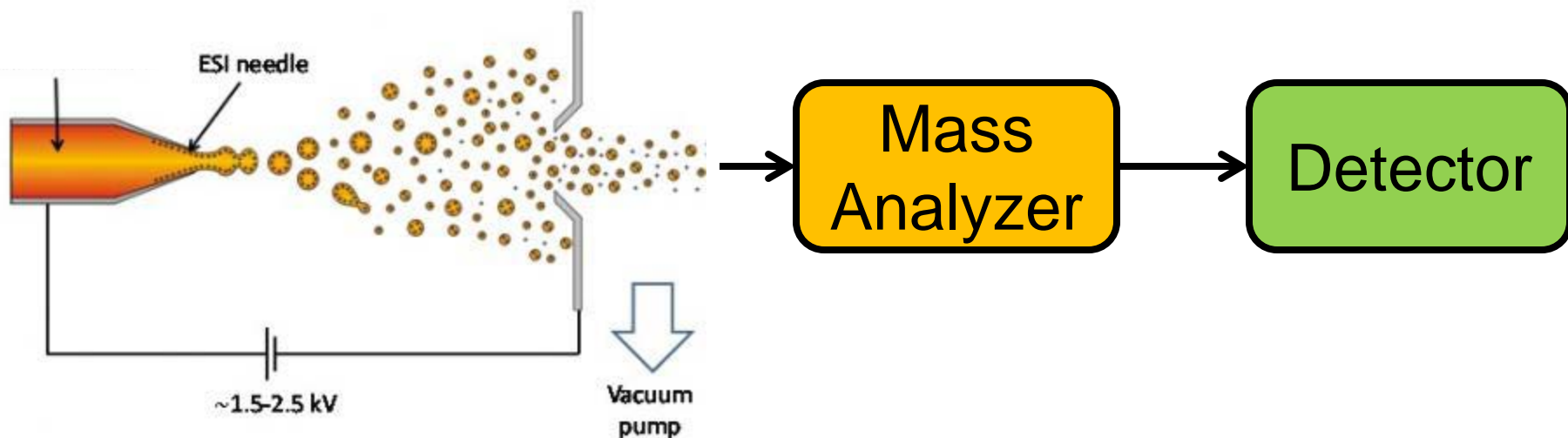
Liquid Chromatography (LC)-MS/MS



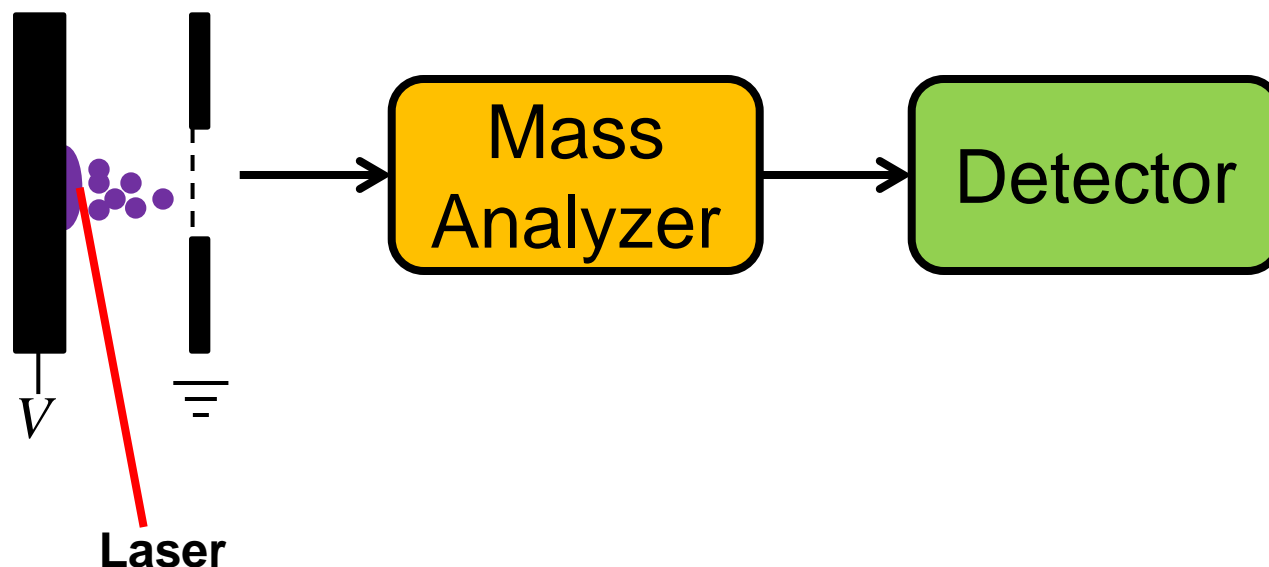
Ion Sources



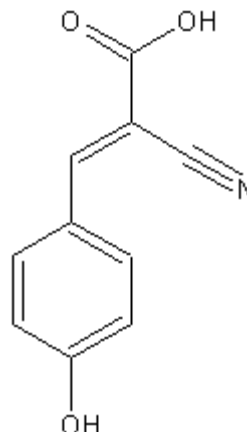
Electrospray



Matrix Assisted Laser Desorption Ionization (MALDI)

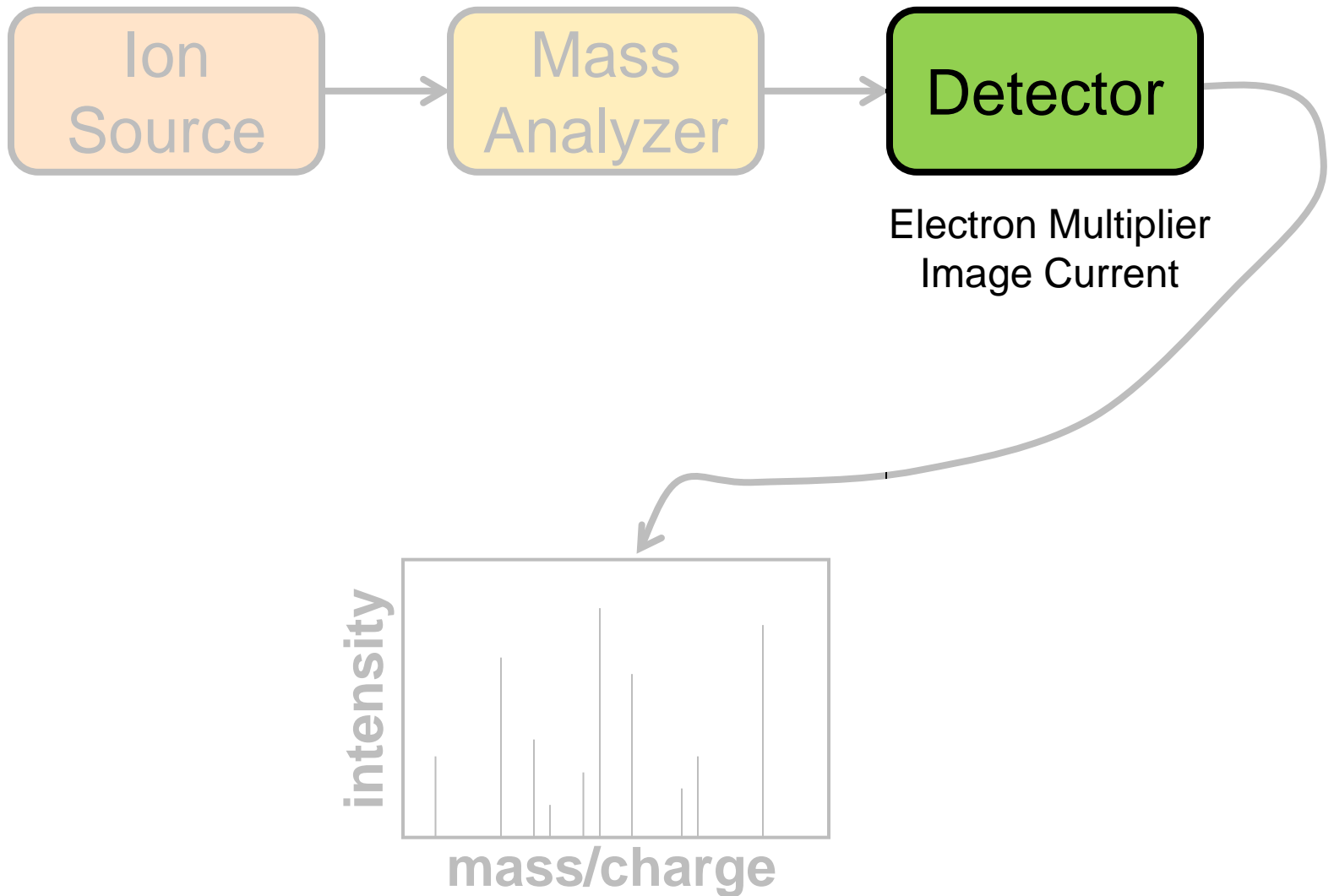


Matrix



alpha-cyano-4-hydroxycinnamic acid

Detectors



Electron Multiplier Detector

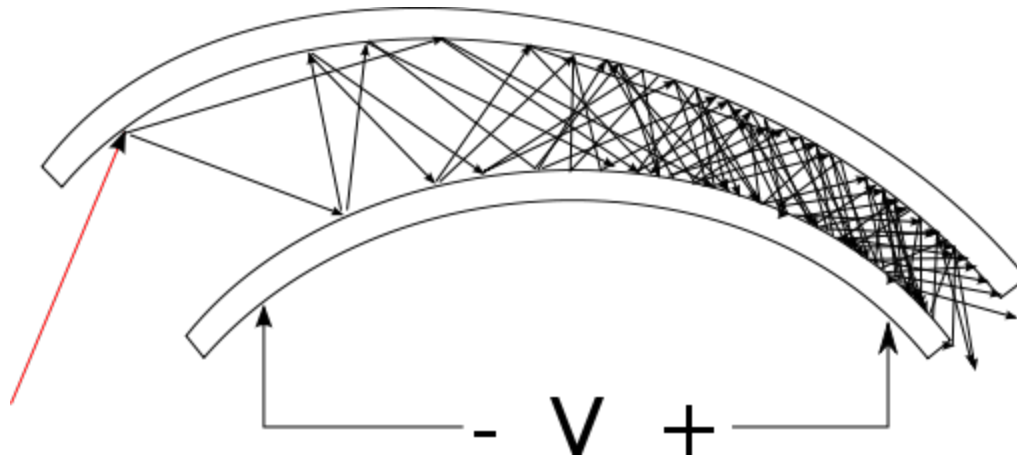
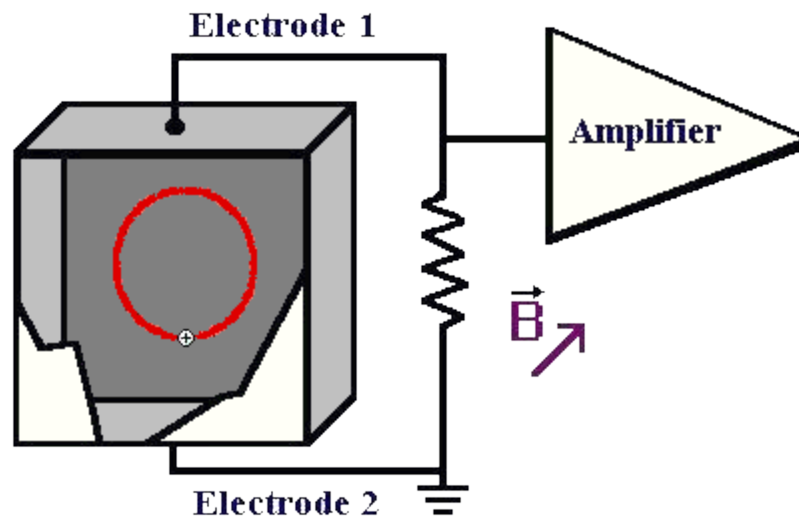
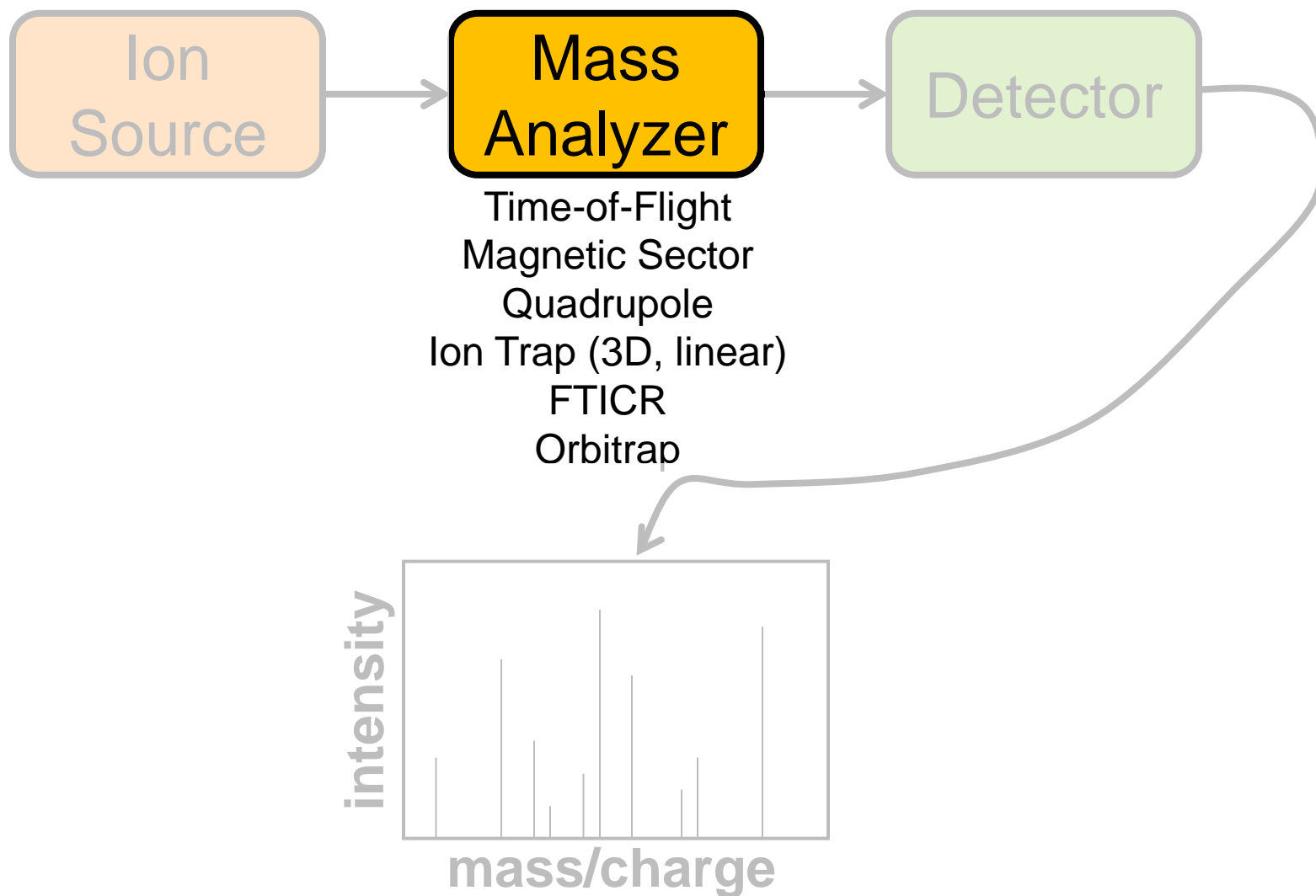


Image Current Detector

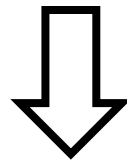


Mass Analyzers



Mass Spectrometry (MS)

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

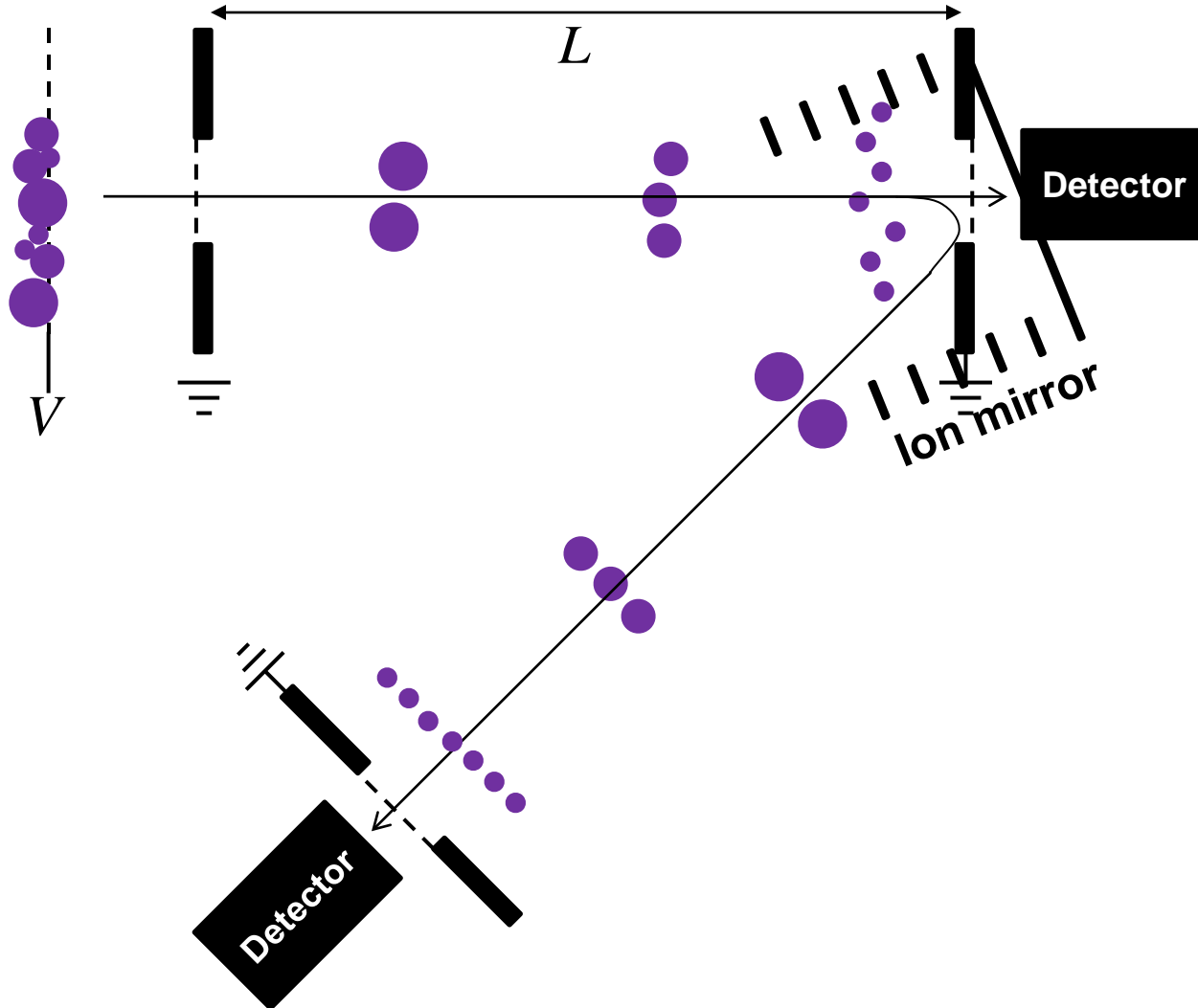


$$\boxed{\frac{m}{z}} \frac{d\overline{v}}{dt} = \overline{E} + \overline{v} \times \overline{B}$$

Time-of-Flight Mass Spectrometry

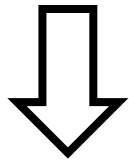


Time-of-Flight



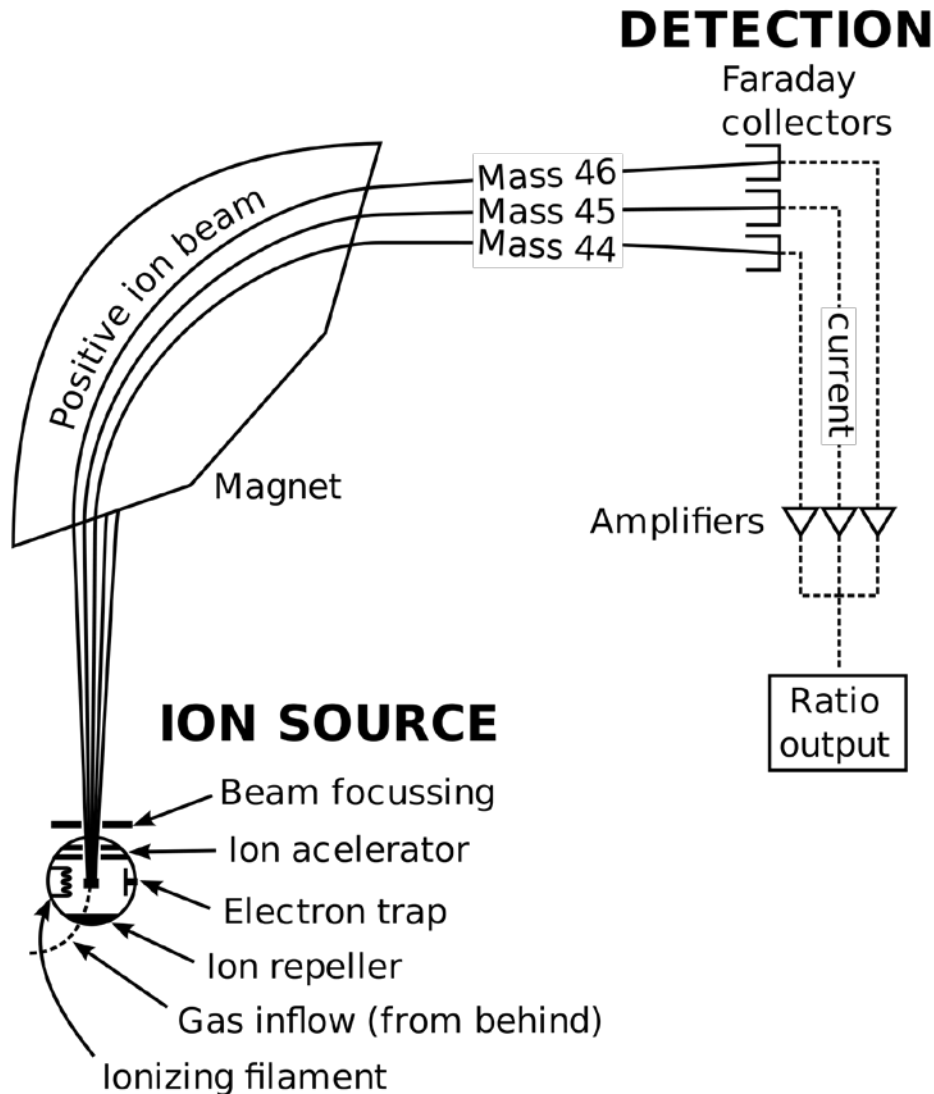
$$zV = \frac{mv^2}{2}$$

$$L = vt$$



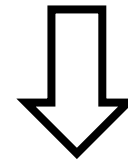
$$t = \frac{L}{\sqrt{2V}} \sqrt{\frac{m}{z}}$$

Magnetic Sector



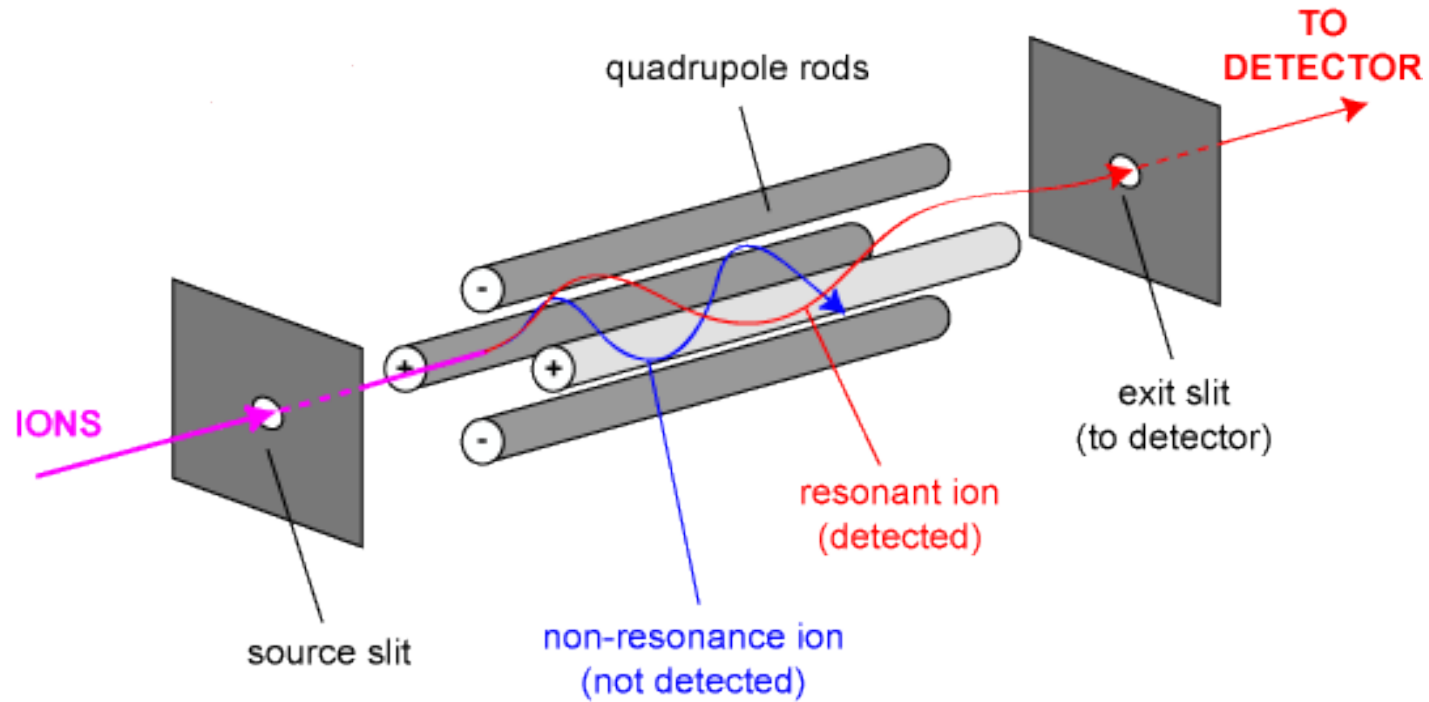
$$\overline{F} = \frac{mv^2}{R} = zvB$$

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



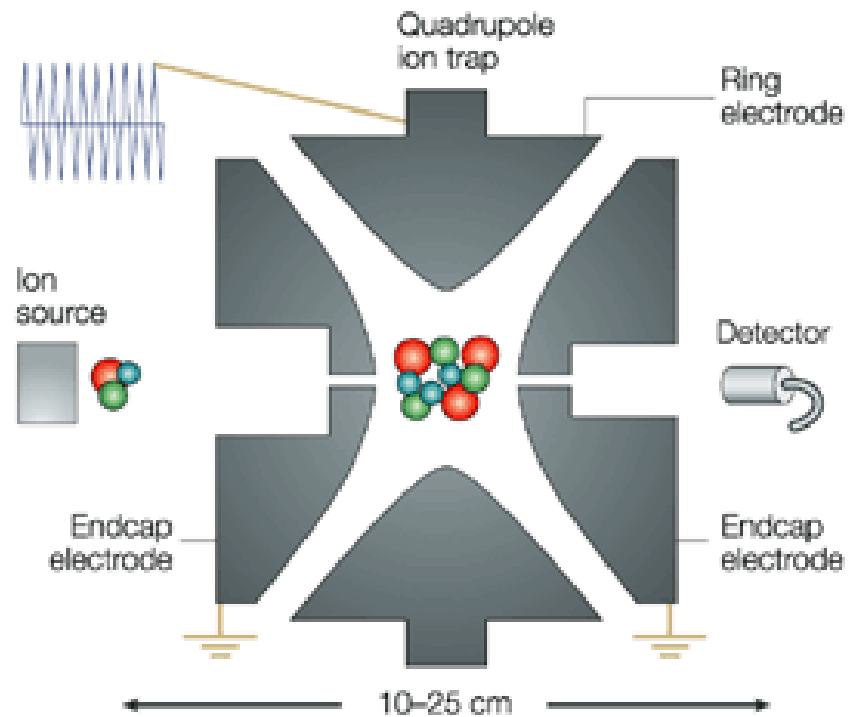
$$R = \sqrt{\frac{m}{z}} \sqrt{\frac{2V}{B}}$$

Quadrupole Mass Filter



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

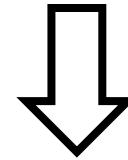
Ion Trap



Fourier transform ion cyclotron resonance



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



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

Orbitrap

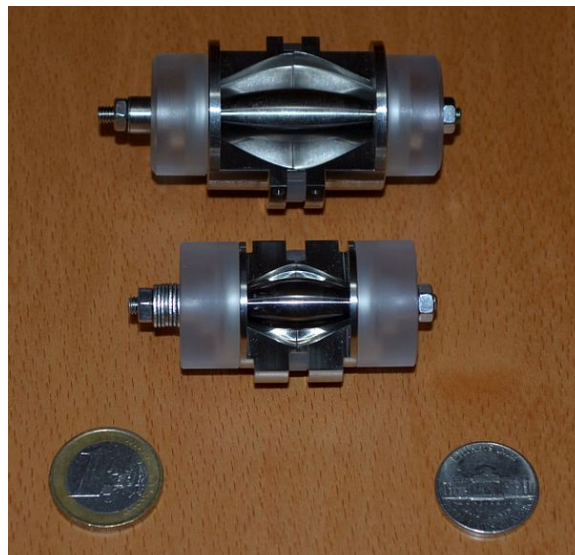
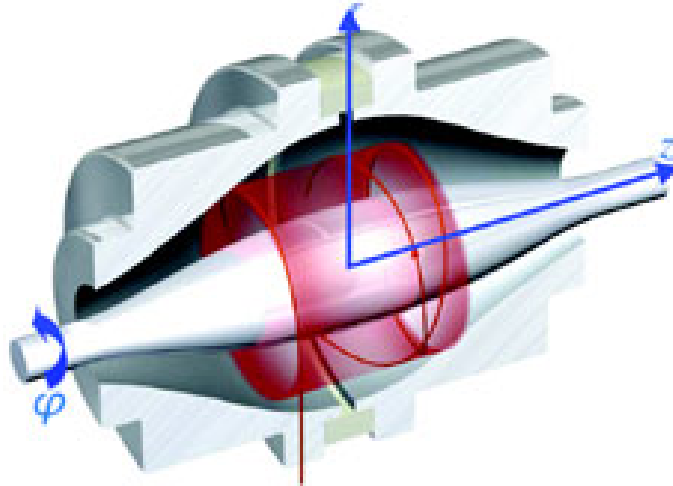
- Characteristic frequencies:

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

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

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

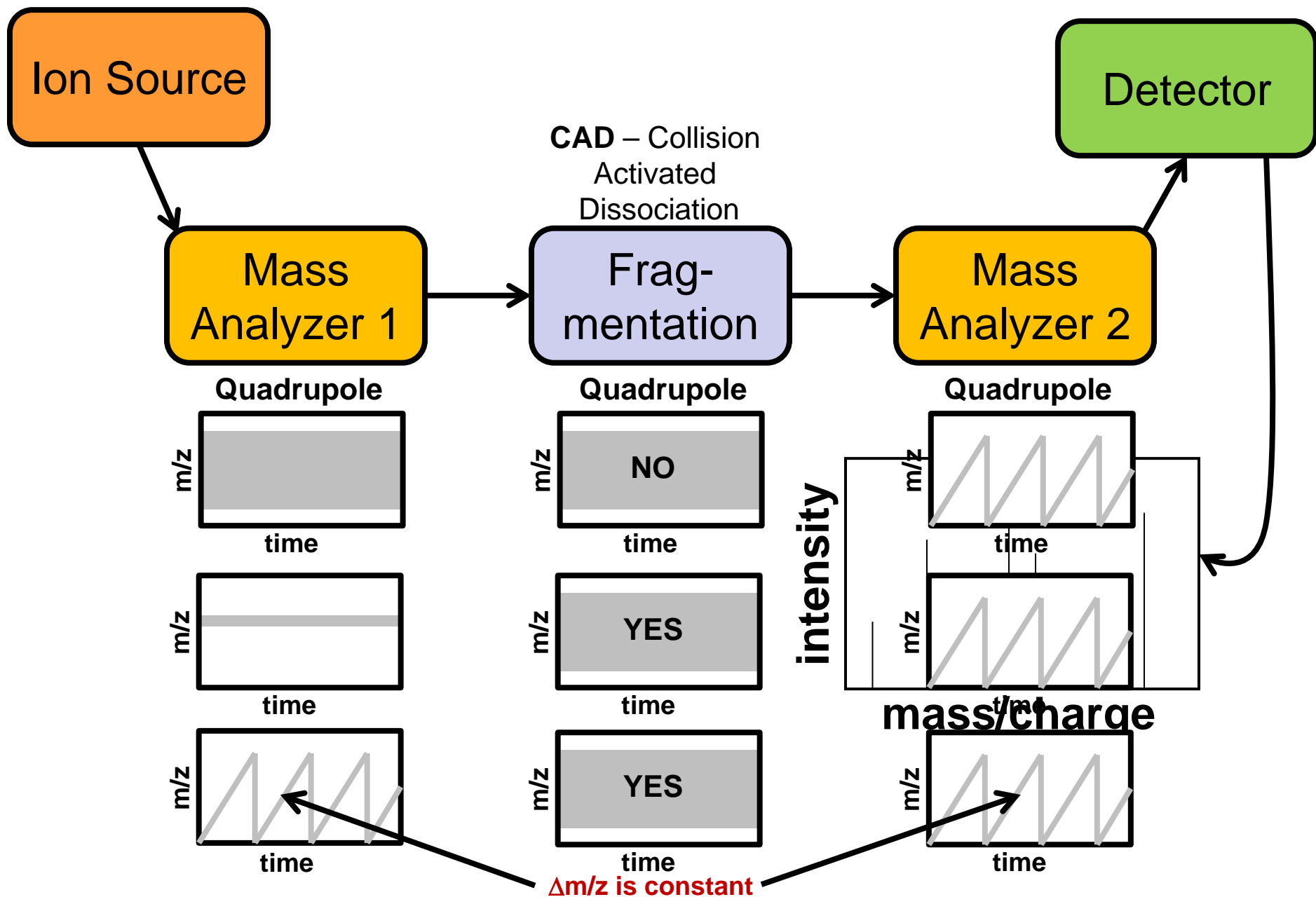
$$\omega_z = \sqrt{\frac{k}{m/z}}$$



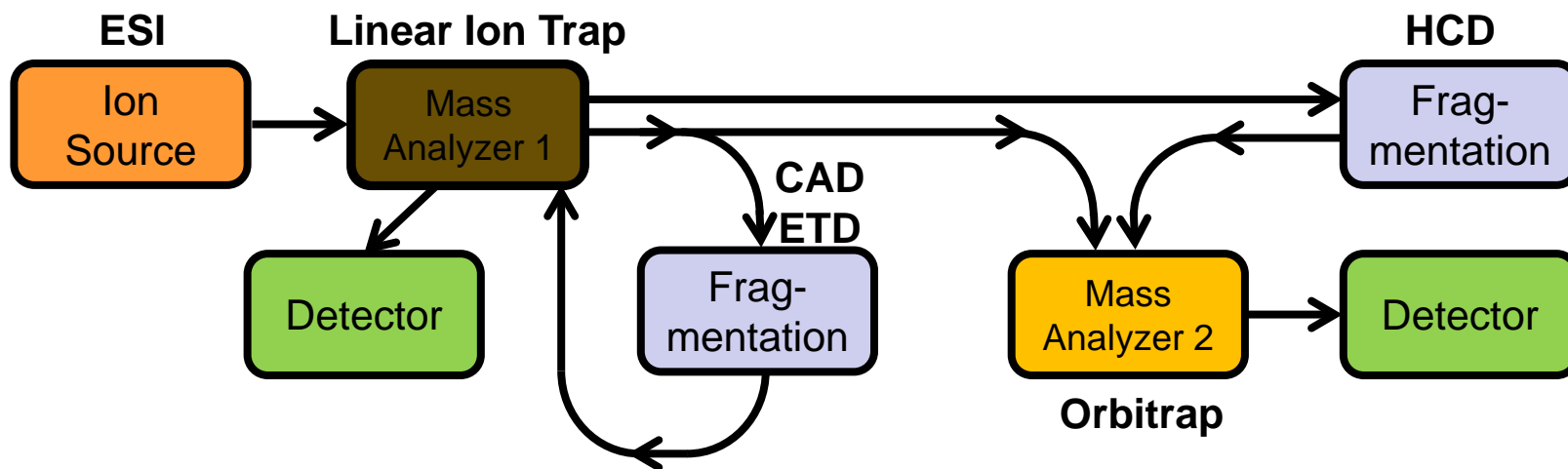
Quadrupole Time-of-Flight Mass Spectrometer

[Video](#)

Triple Quadrupole



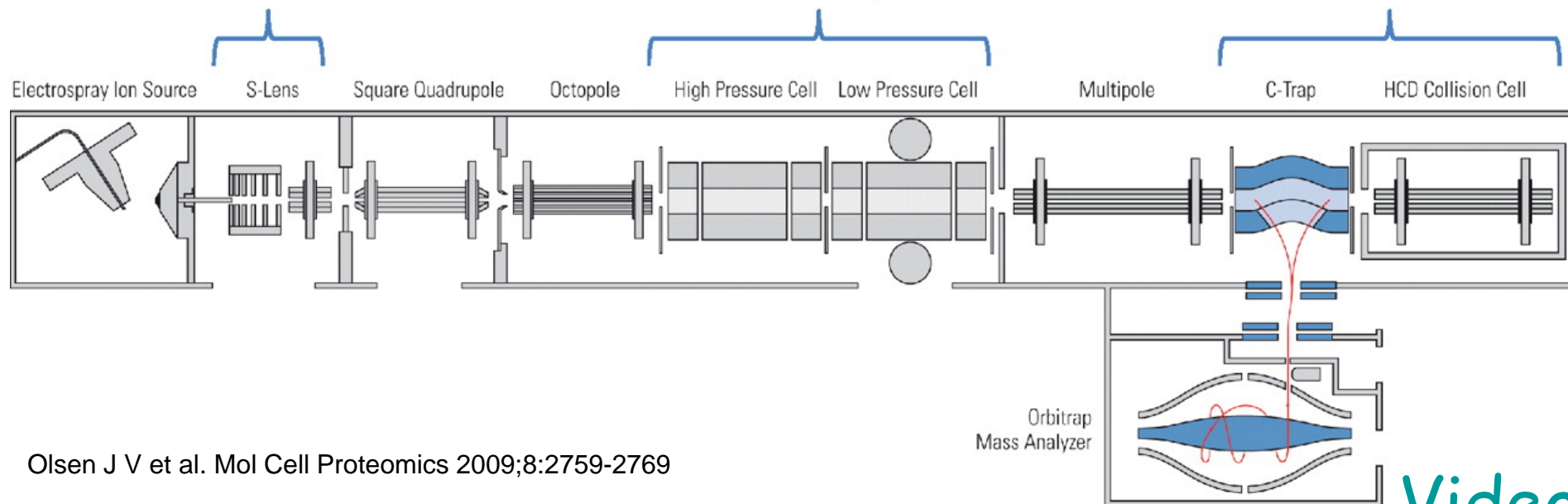
Linear Ion Trap / Orbitrap



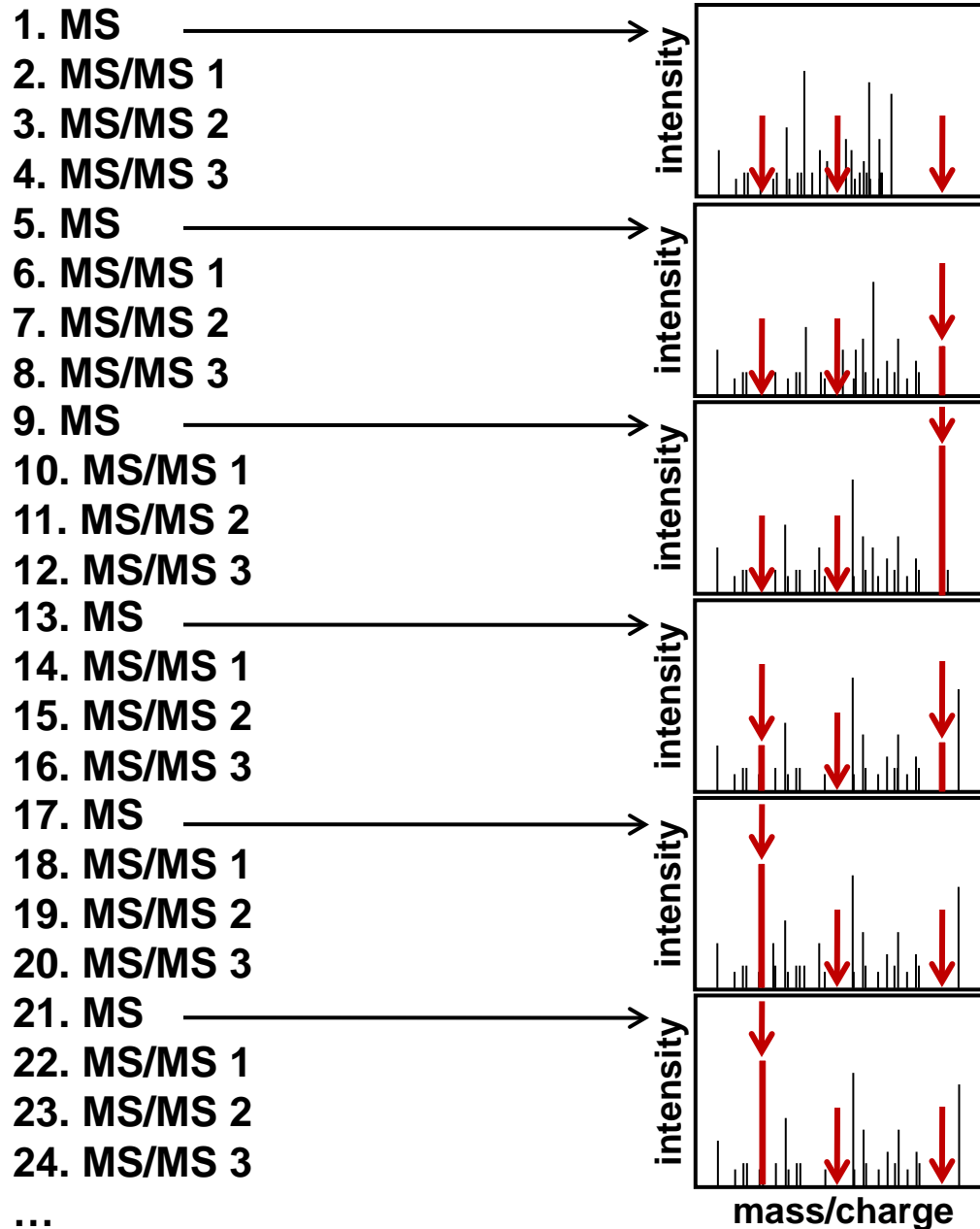
A. Stacked Ring Ion Guide

B. Dual linear ion trap

C. Combo C-trap/
HCD collision cell

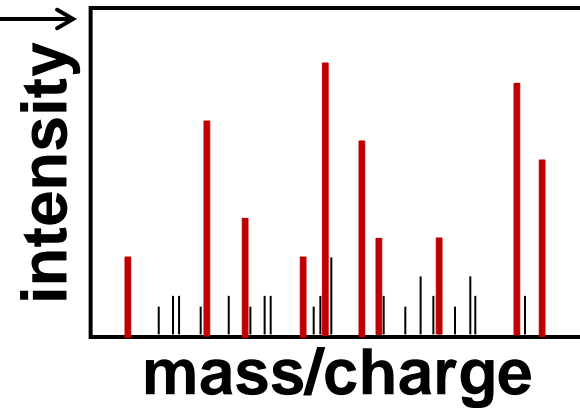


Data Independent Acquisition



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

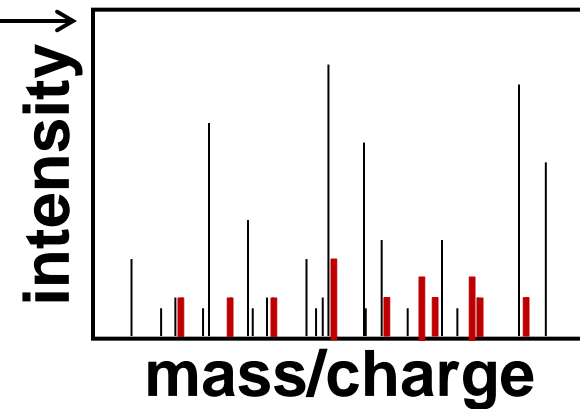
19. MS/MS 7

20. MS/MS 8

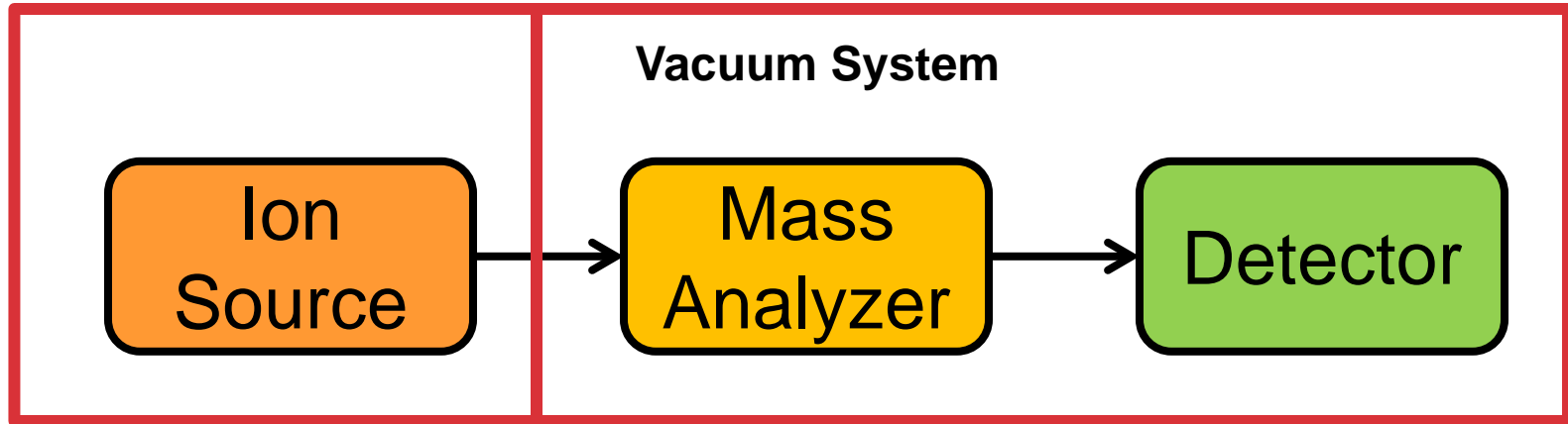
21. MS/MS 9

22. MS/MS 10

...



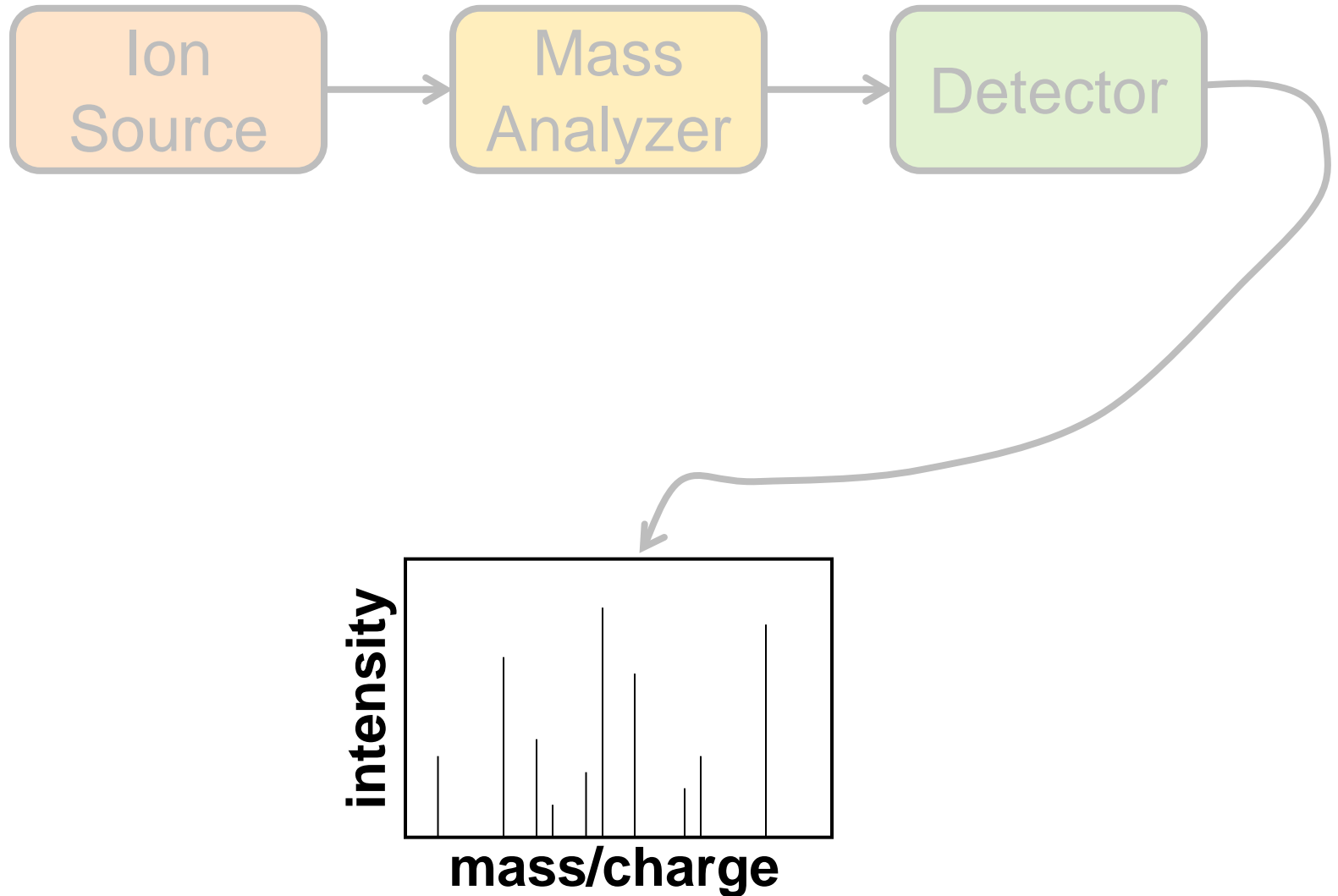
Vacuum System



Atmosphere



Mass Spectrometry Data



Mass Spectrometry Data

Dimensions:

Time

Peptide m/z

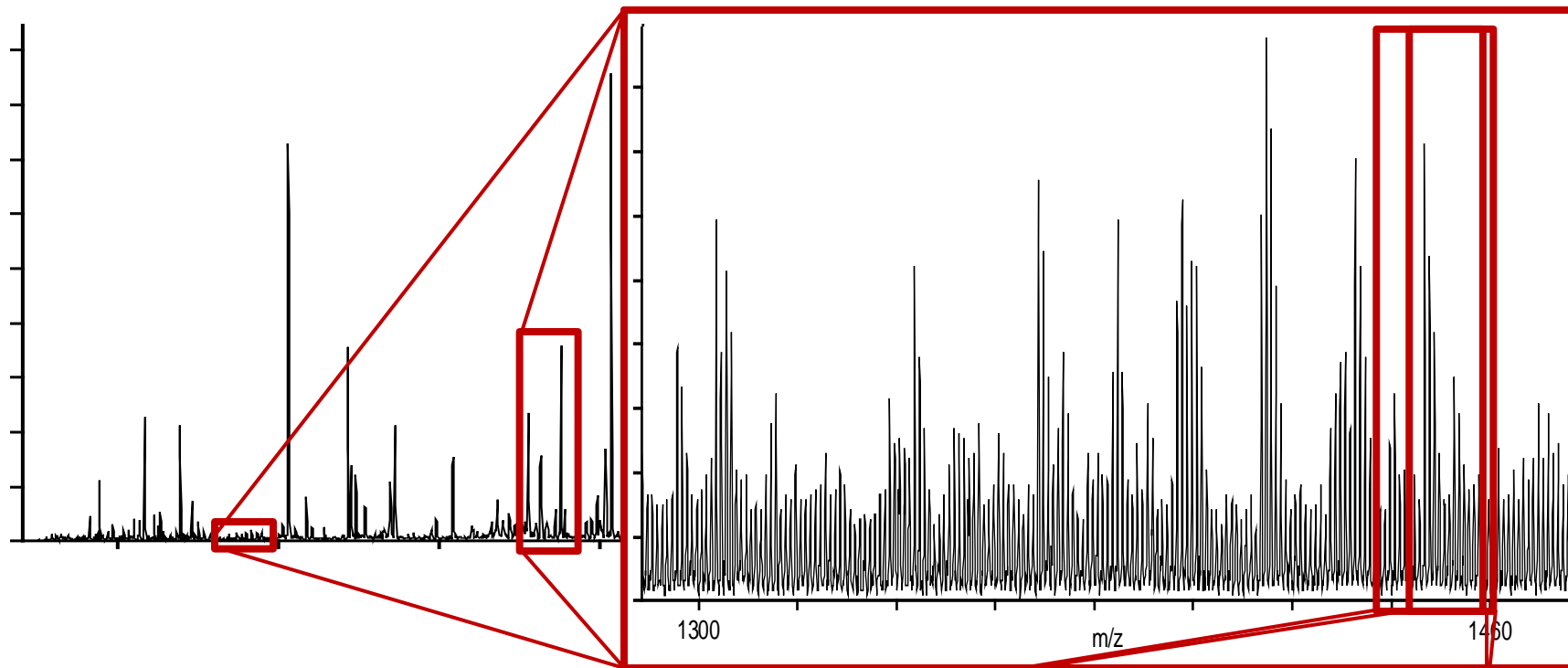
Peptide Intensity

Peptide fragment m/z

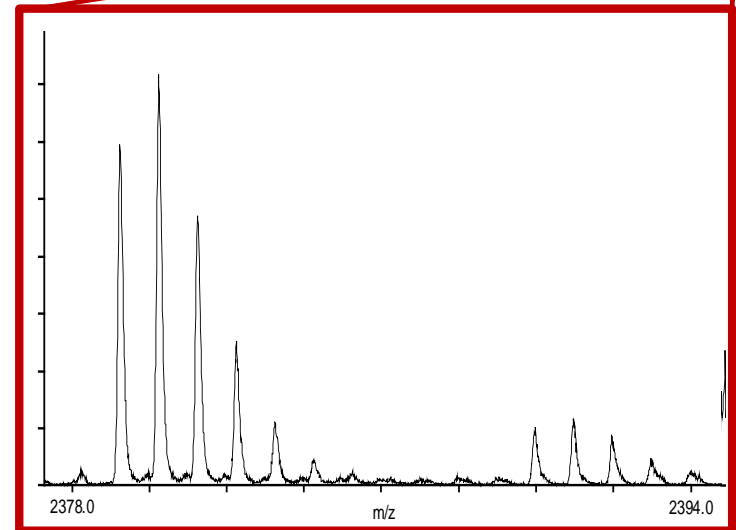
Peptide fragment intensity

...

Example data - MALDI-TOF

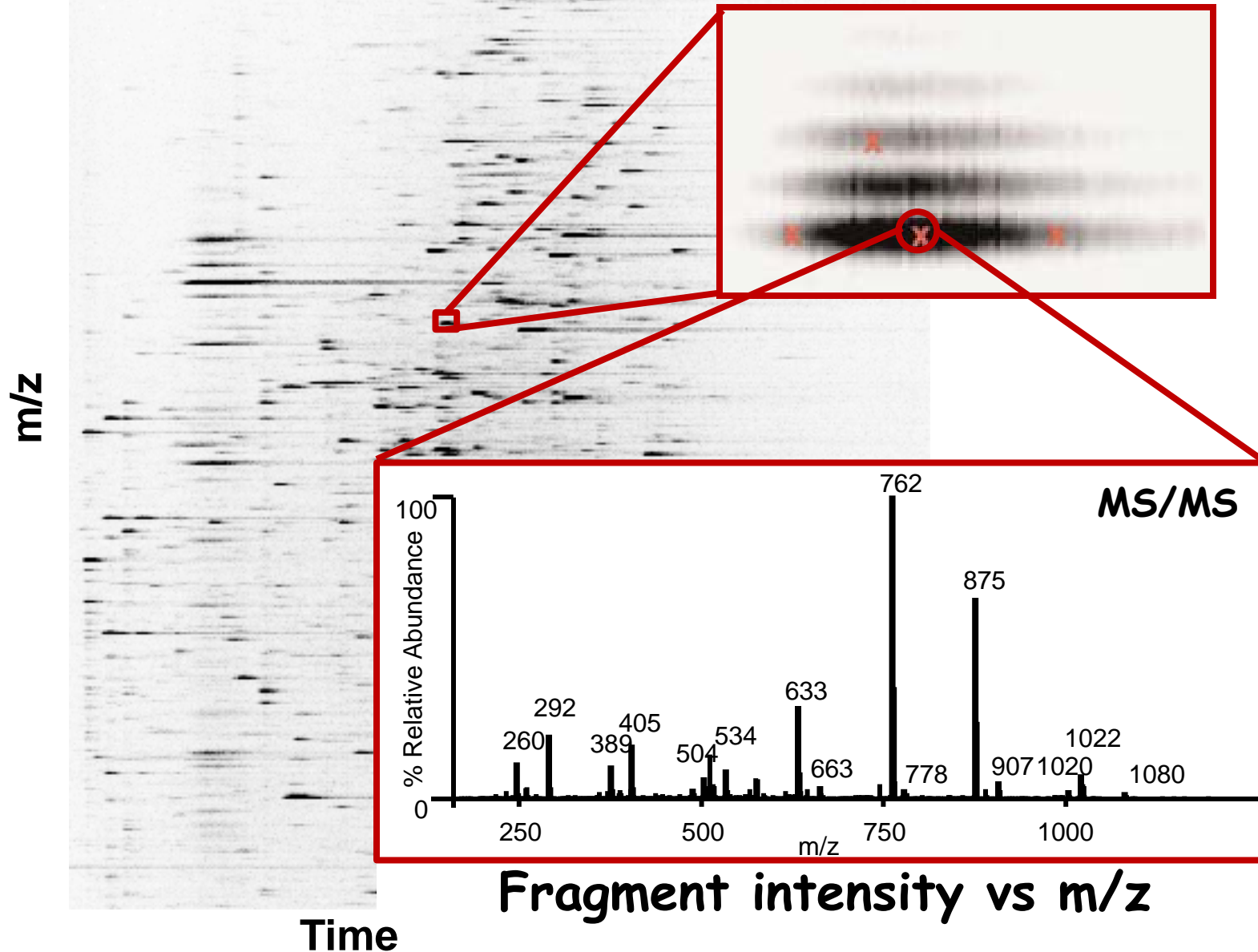


Peptide intensity vs m/z



Example data - ESI-LC-MS/MS

Peptide intensity vs m/z vs time

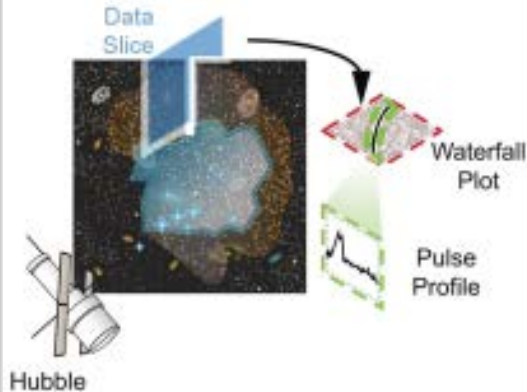


Slice - Scalable Data Sharing for Remote Mass Informatics

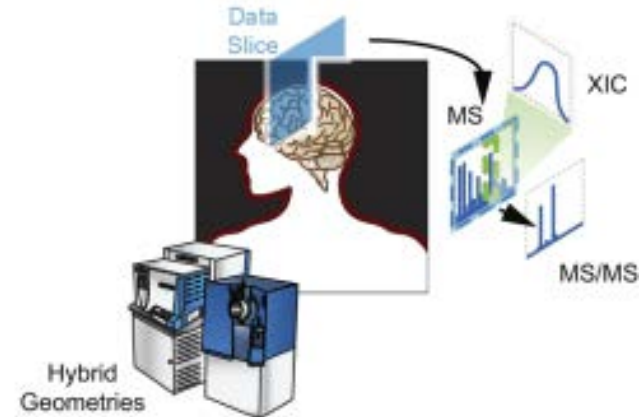


Developed by Manor Askenazi
slice.ionomix.com

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

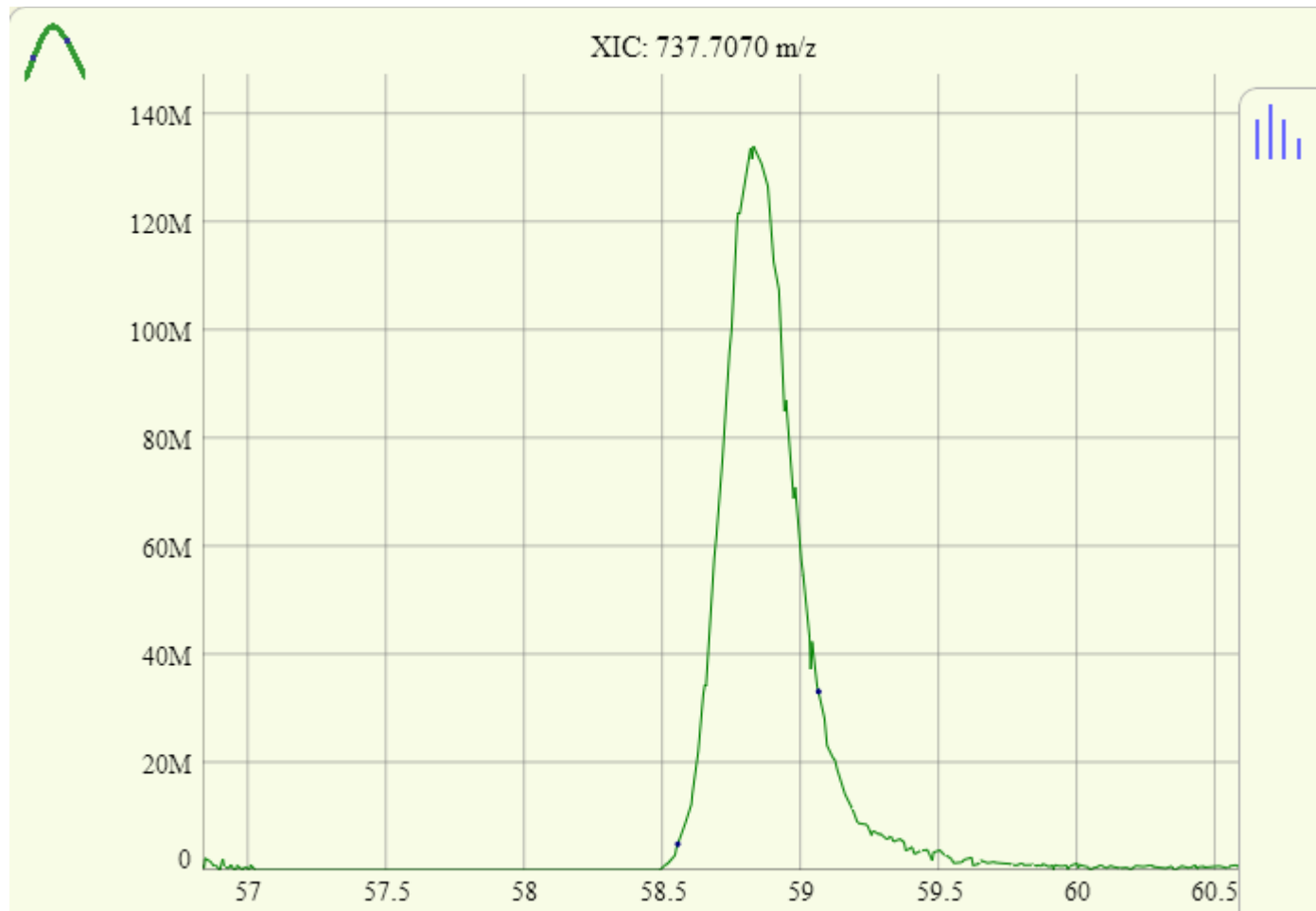
Slice 

=> 

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		✓

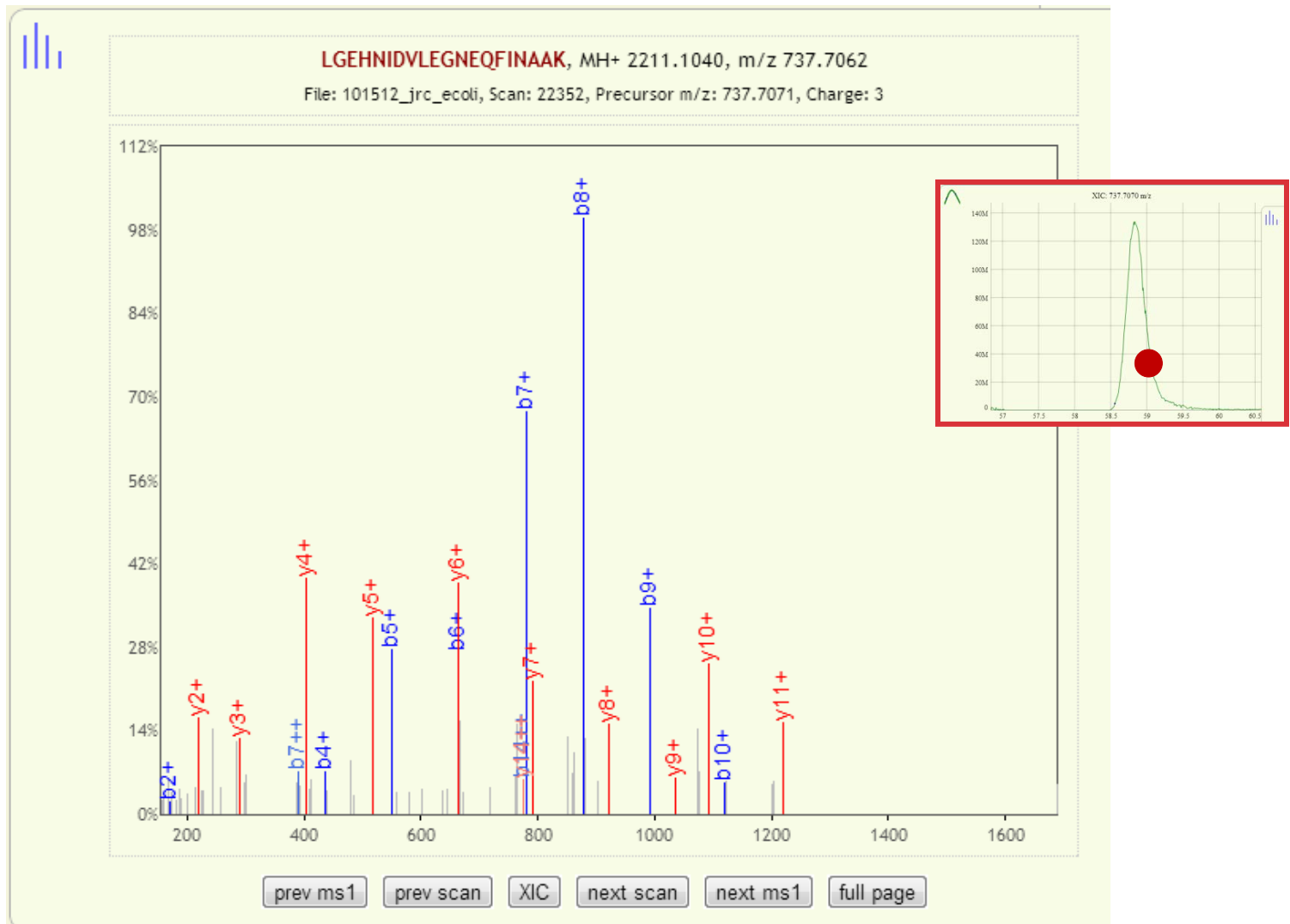
fenyolab.ionomix.com

Example Mass Spectrometry Data

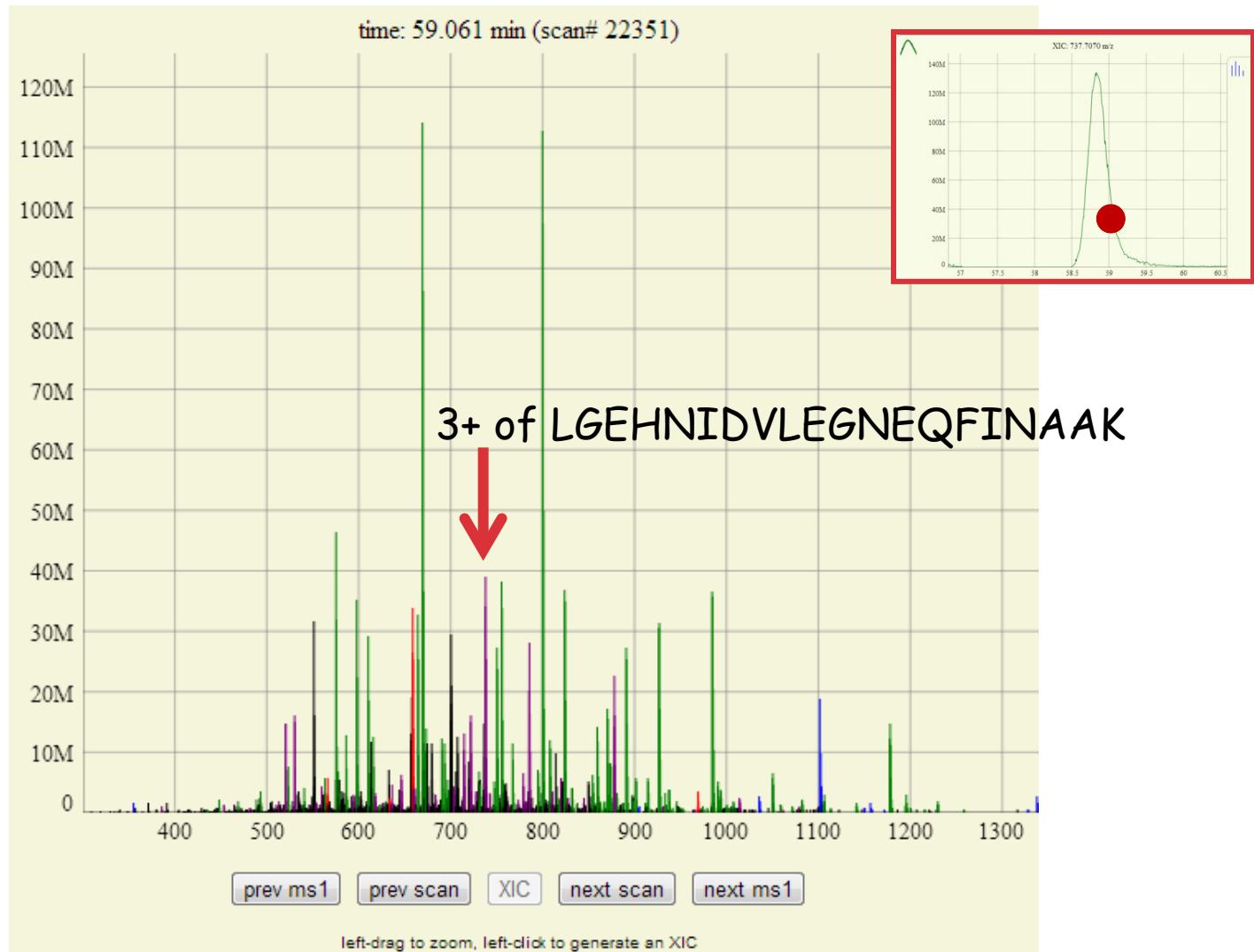


Peptide intensity vs time
For 737.707 m/z which corresponds to
3+ of LGEHNIDVLEGNEQFINAAK

Example Mass Spectrometry Data

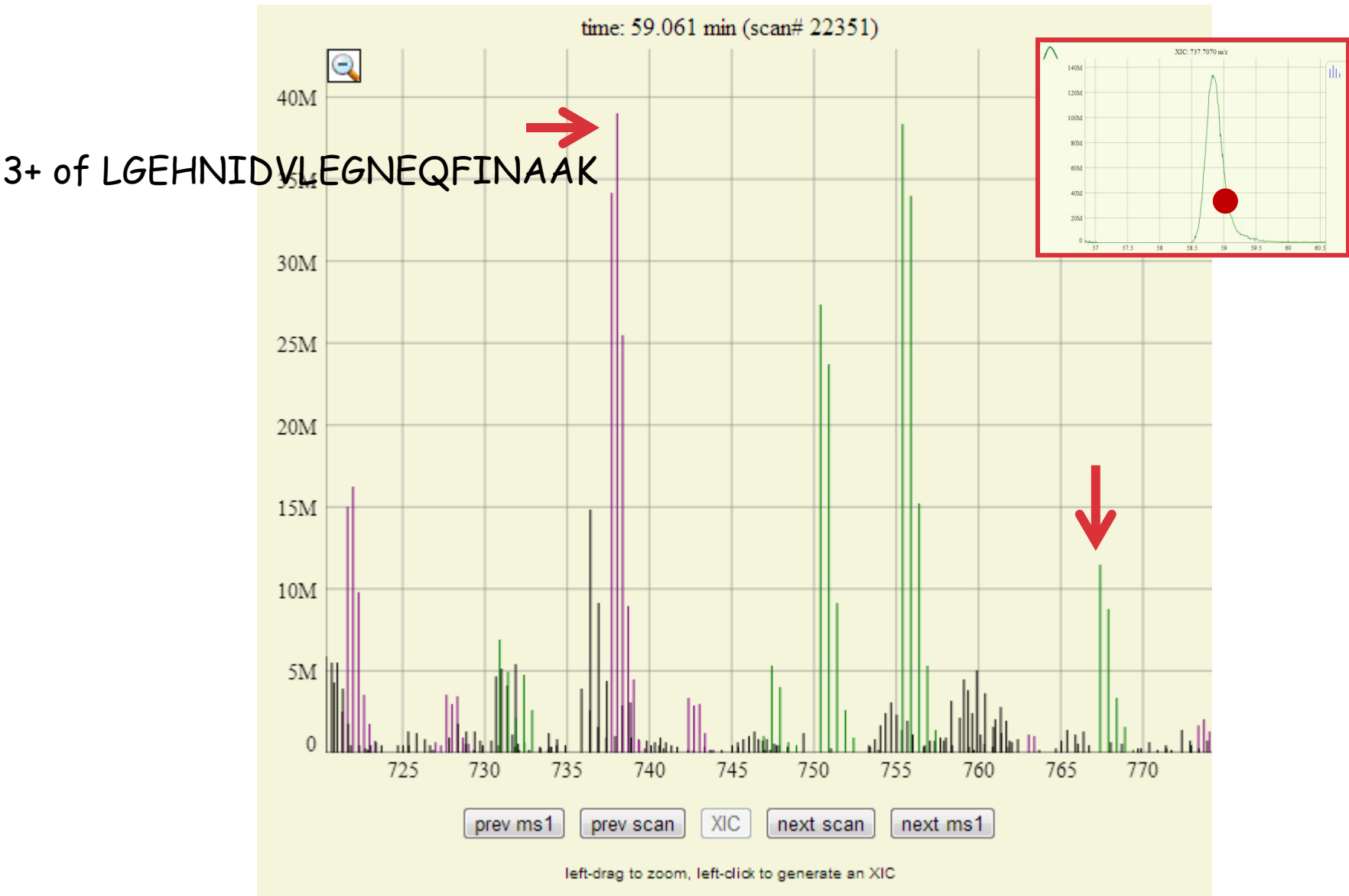


Example Mass Spectrometry Data



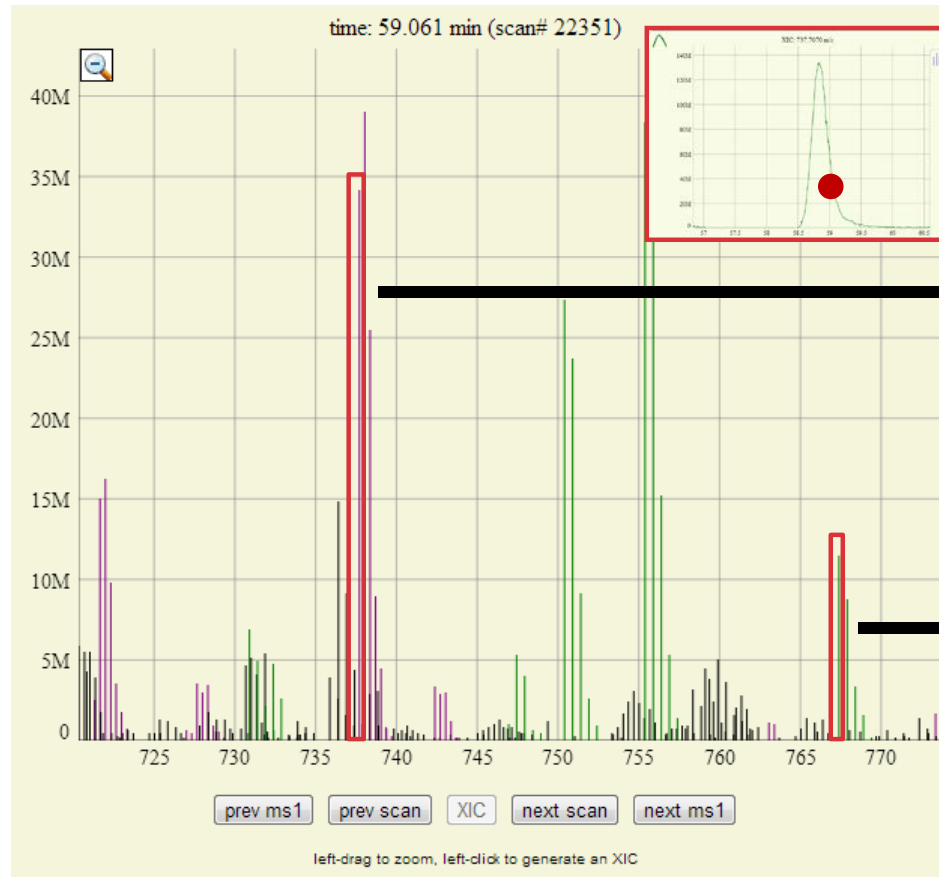
Peptide intensity vs m/z

Example Mass Spectrometry Data

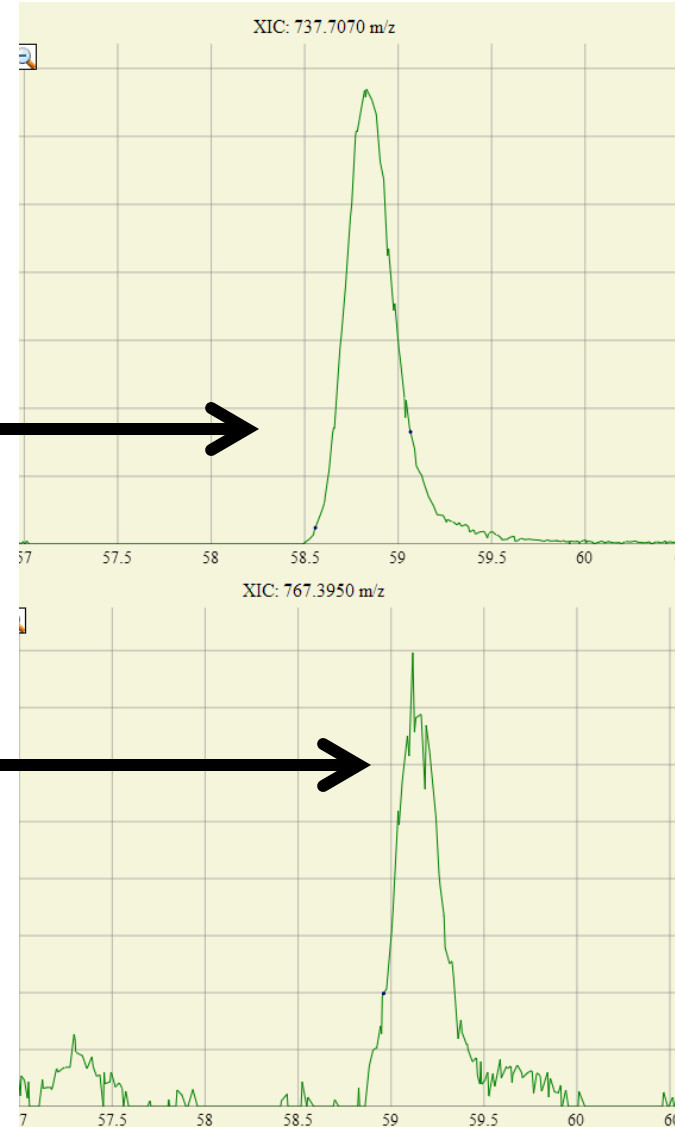


Peptide intensity vs m/z

Example Mass Spectrometry Data



Peptide intensity vs m/z



Peptide intensity vs time

Proteomics Informatics - Overview of Mass spectrometry (Week 2)

