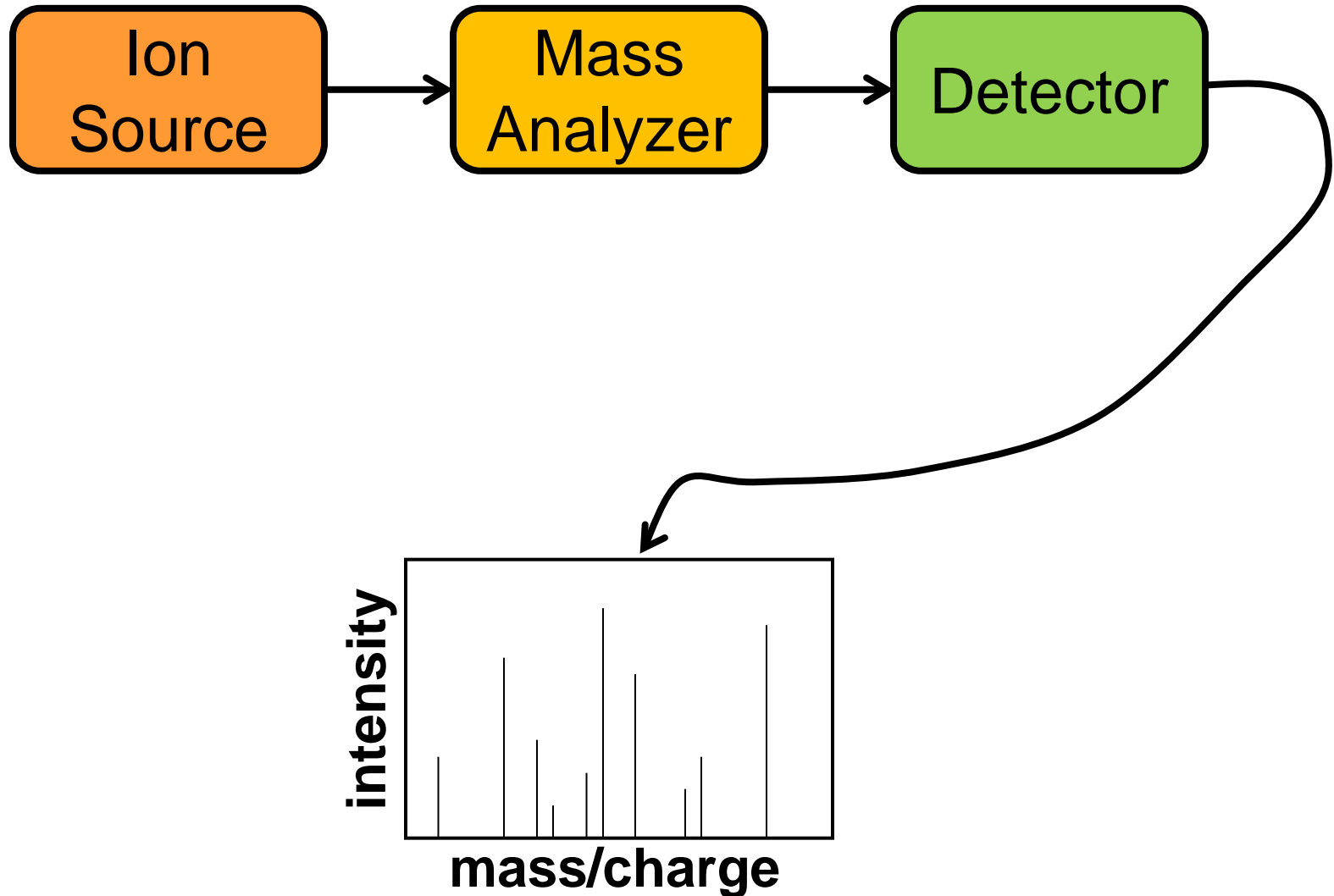
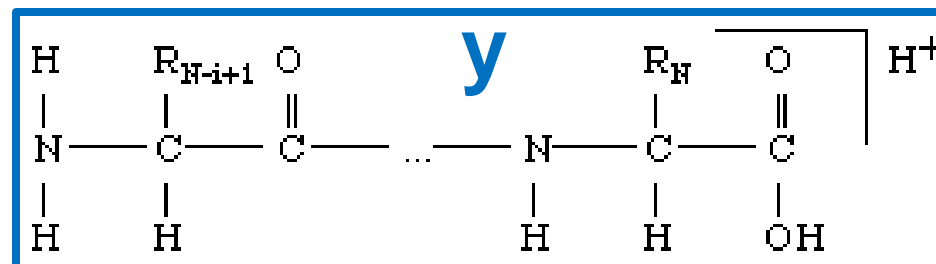
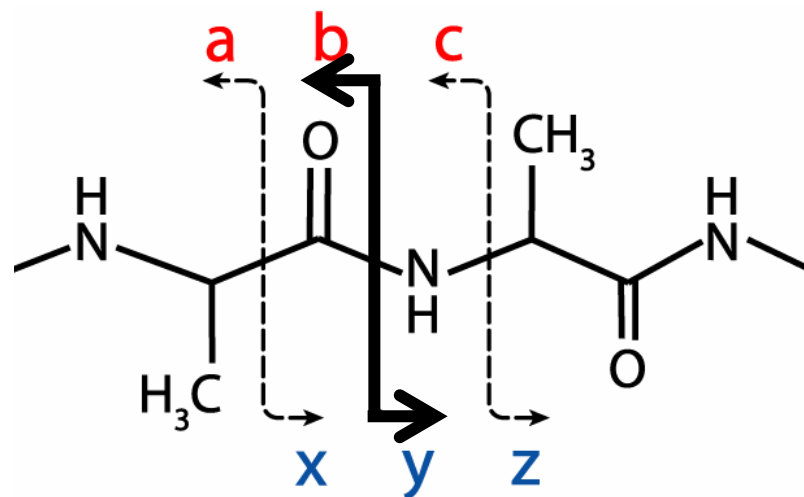
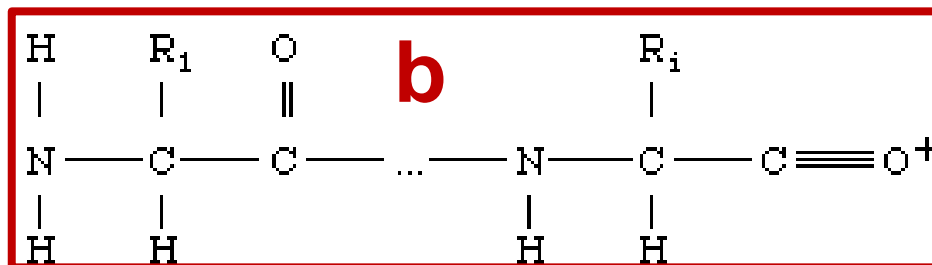


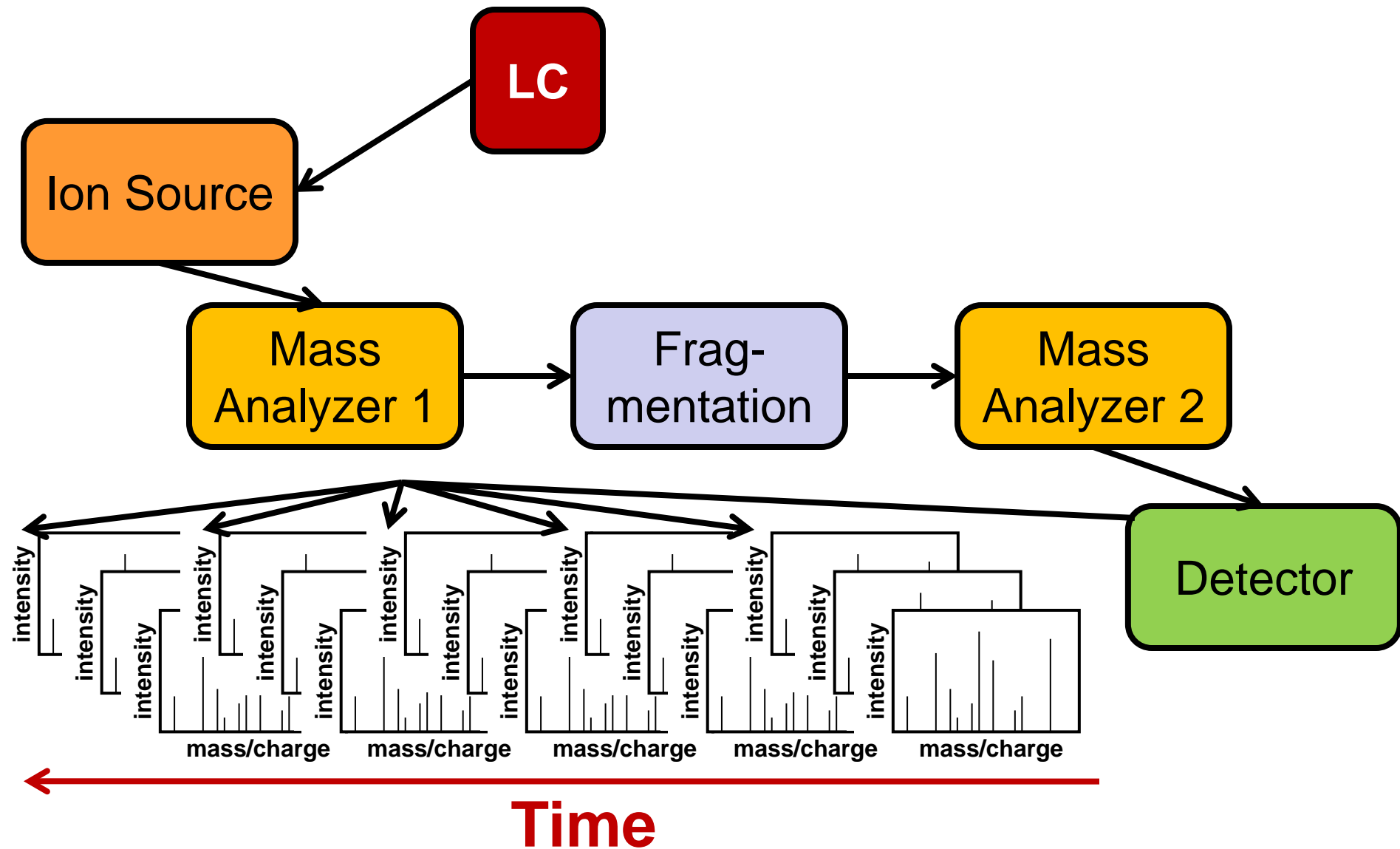
Proteomics Informatics - Overview of Mass spectrometry (Week 2)



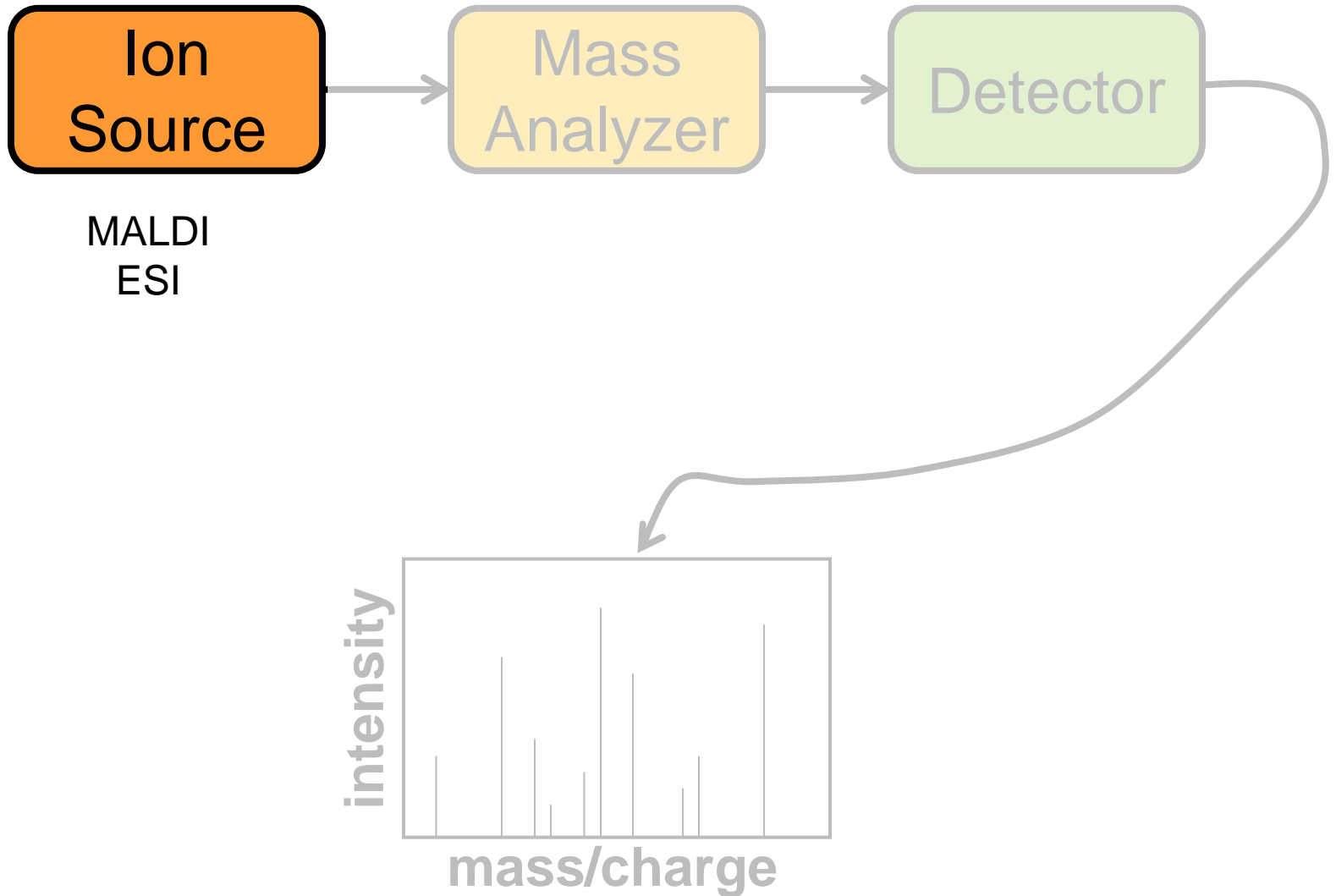
Peptide Fragmentation



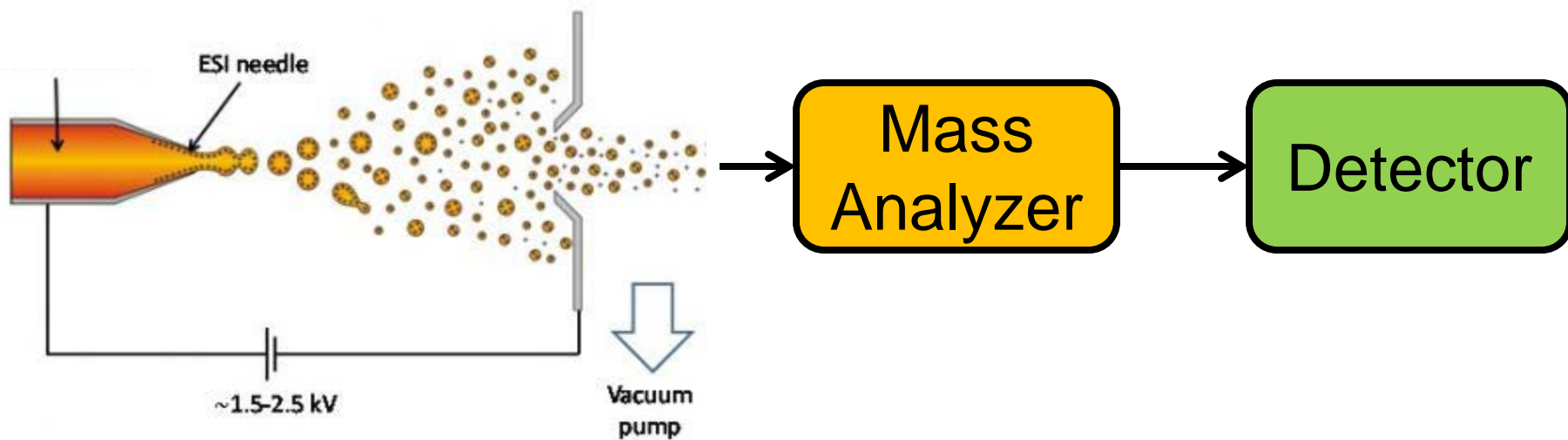
Liquid Chromatography (LC)-MS/MS



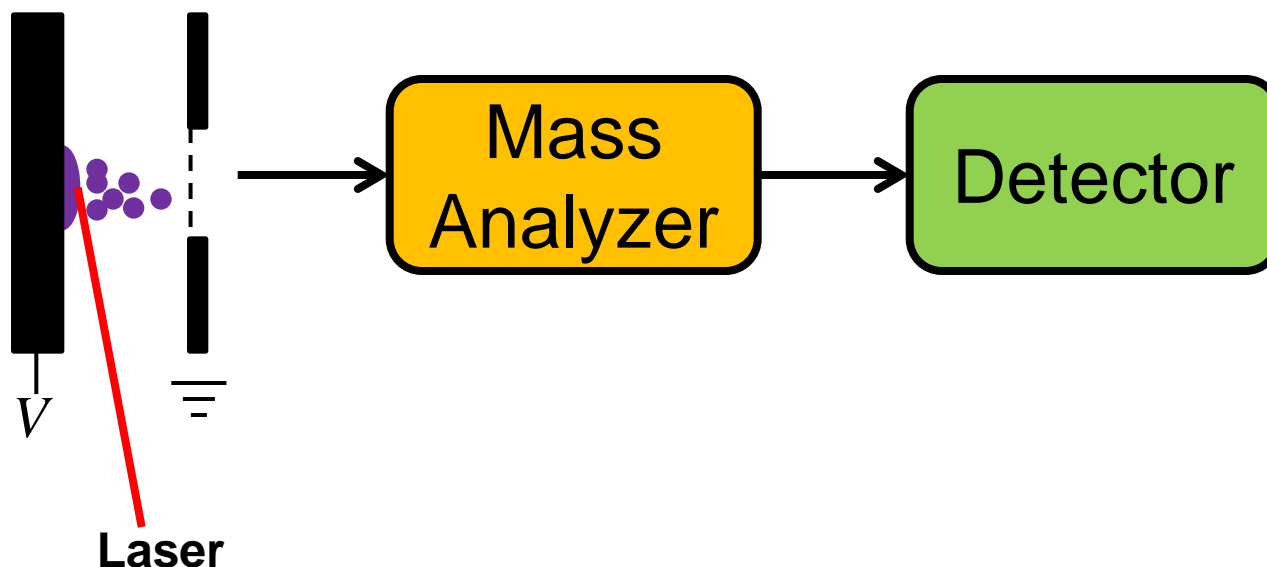
Ion Sources



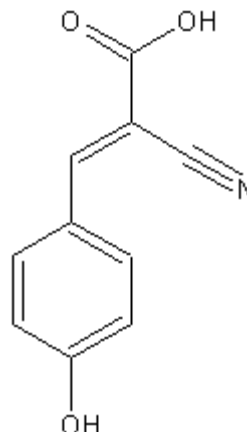
Electrospray



Matrix Assisted Laser Desorption Ionization (MALDI)

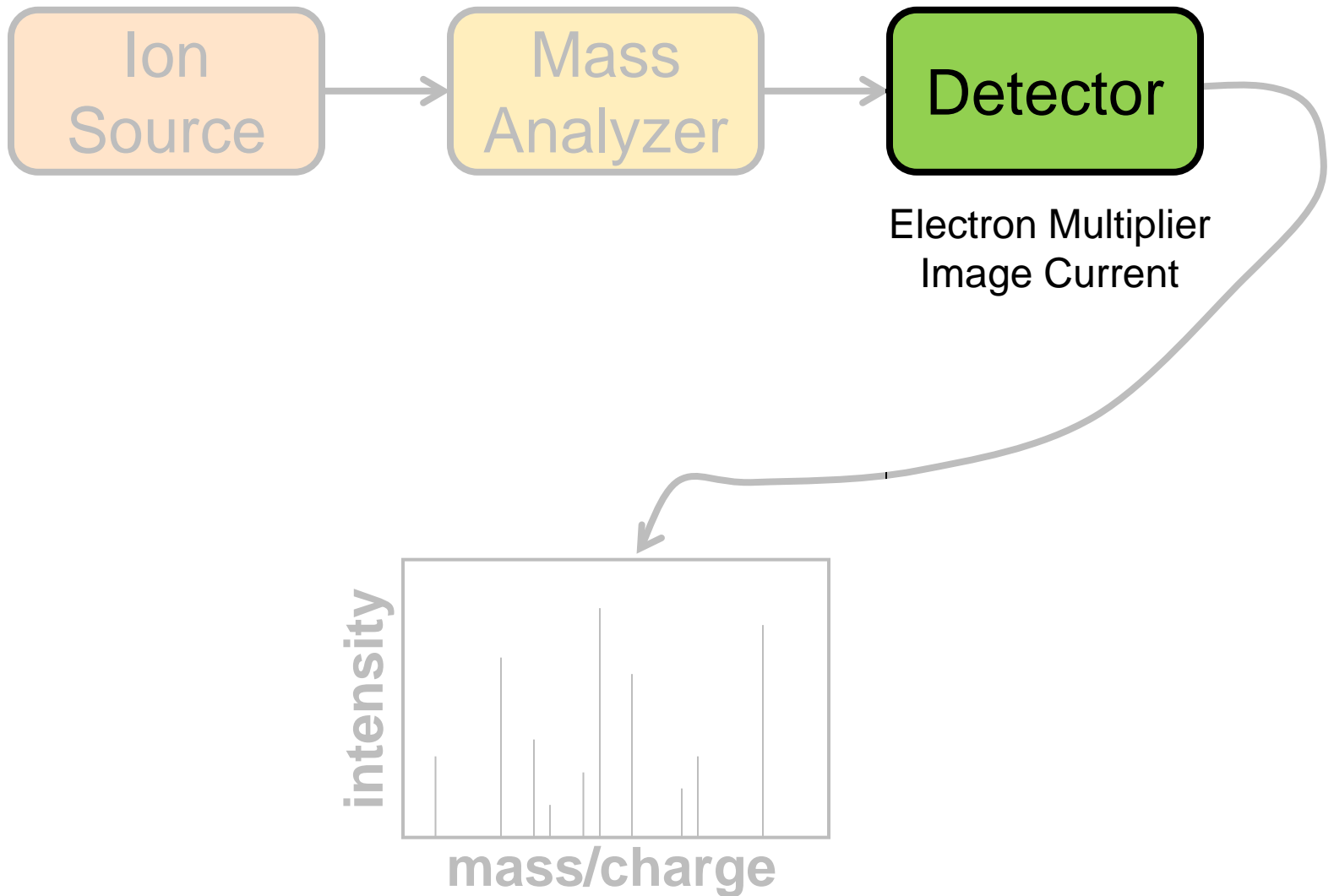


Matrix



alpha-cyano-4-hydroxycinnamic acid

Detectors



Electron Multiplier Detector

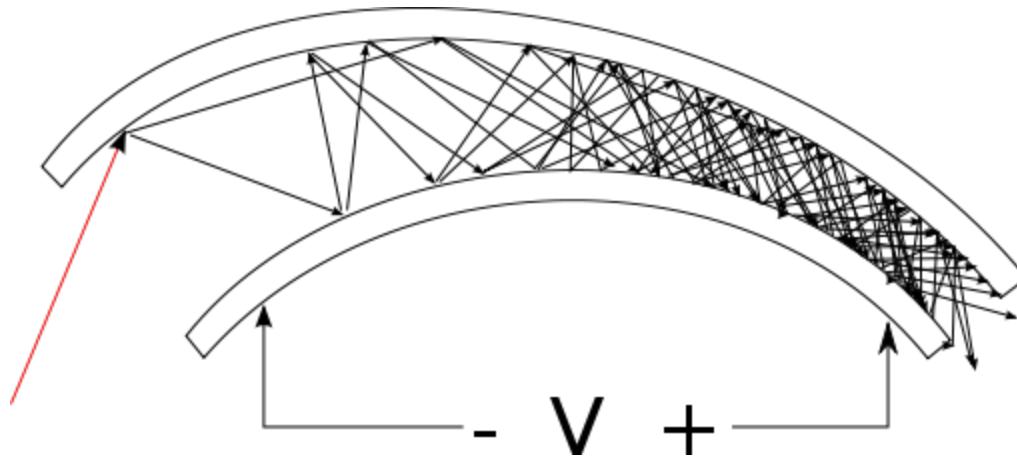
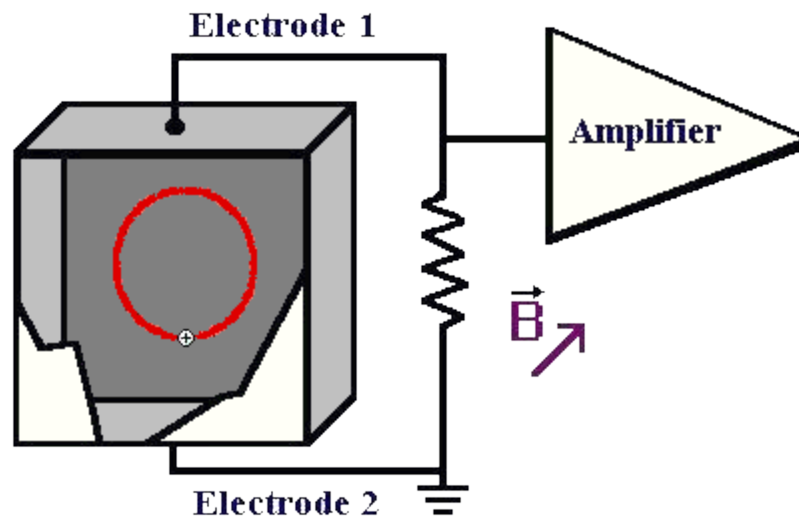
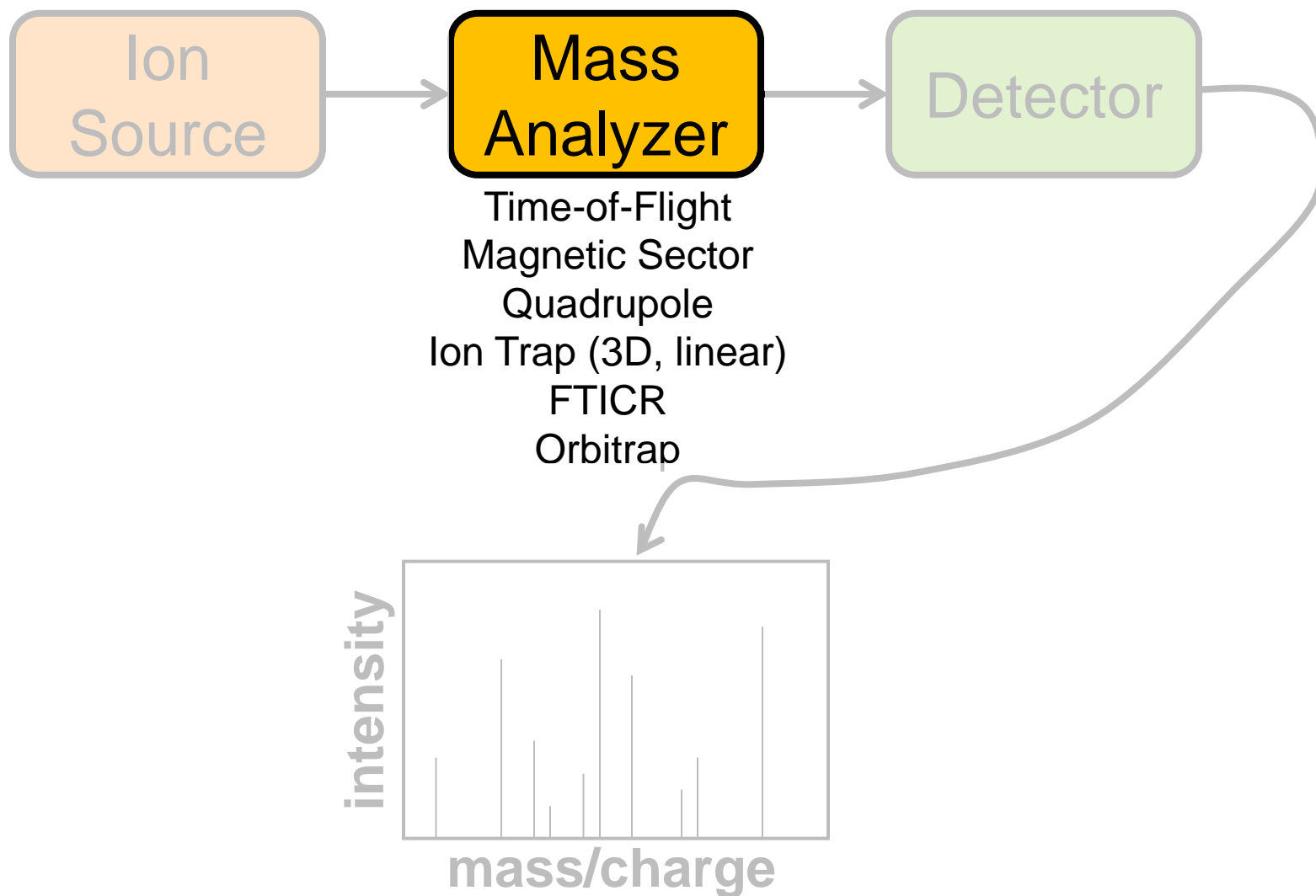


Image Current Detector

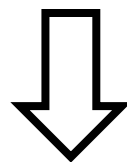


Mass Analyzers



Mass Spectrometry (MS)

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

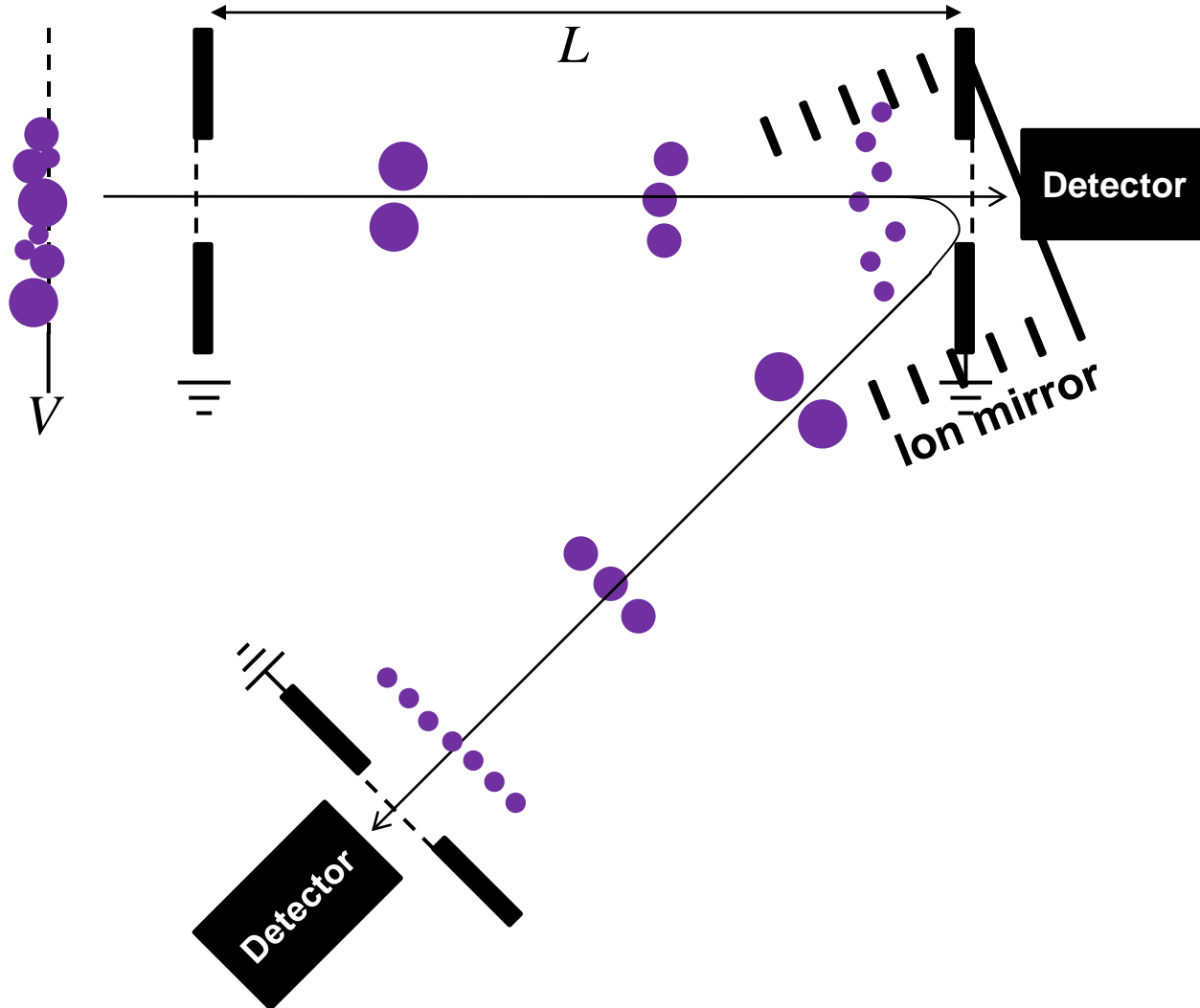


$$\boxed{\frac{m}{z}} \frac{d\overline{v}}{dt} = \overline{E} + \overline{v} \times \overline{B}$$

Time-of-Flight Mass Spectrometry

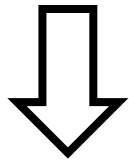


Time-of-Flight



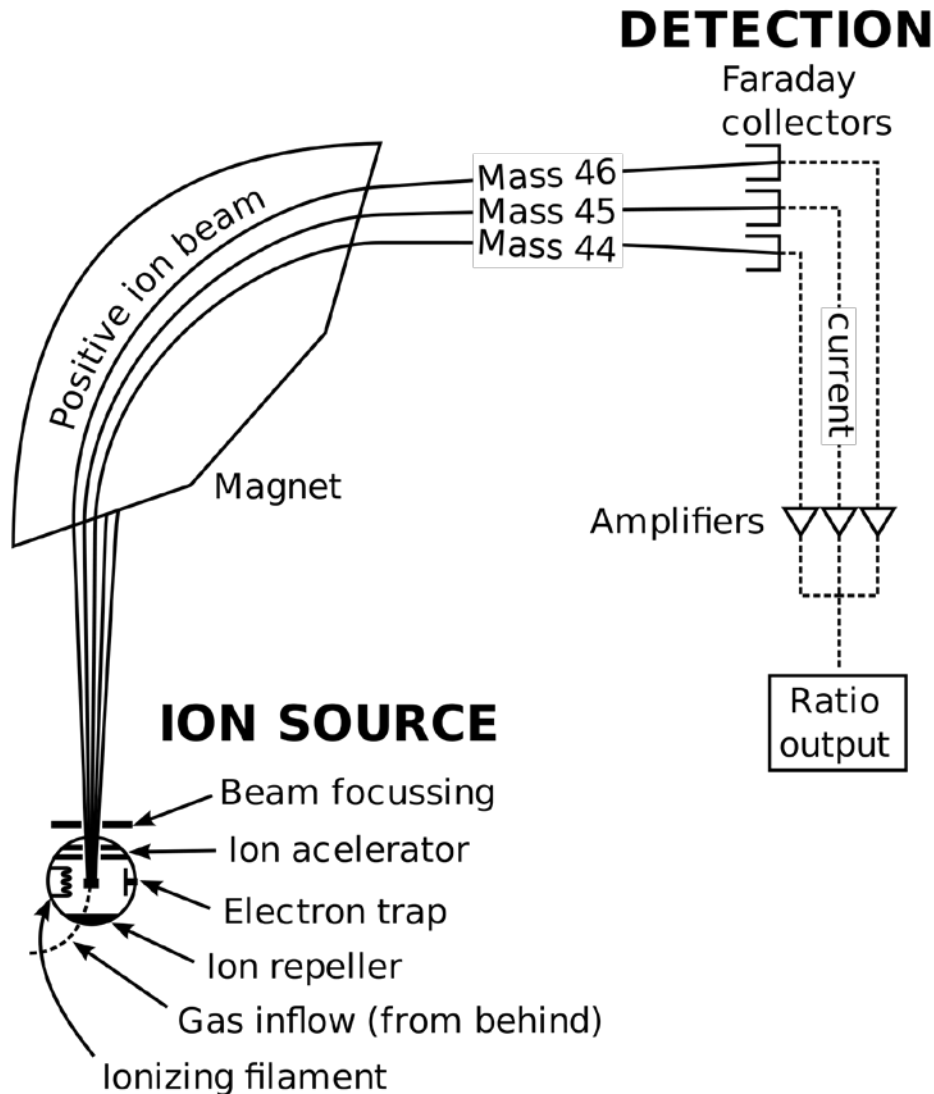
$$zV = \frac{mv^2}{2}$$

$$L = vt$$



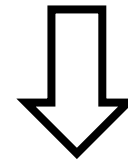
$$t = \frac{L}{\sqrt{2V}} \sqrt{\frac{m}{z}}$$

Magnetic Sector



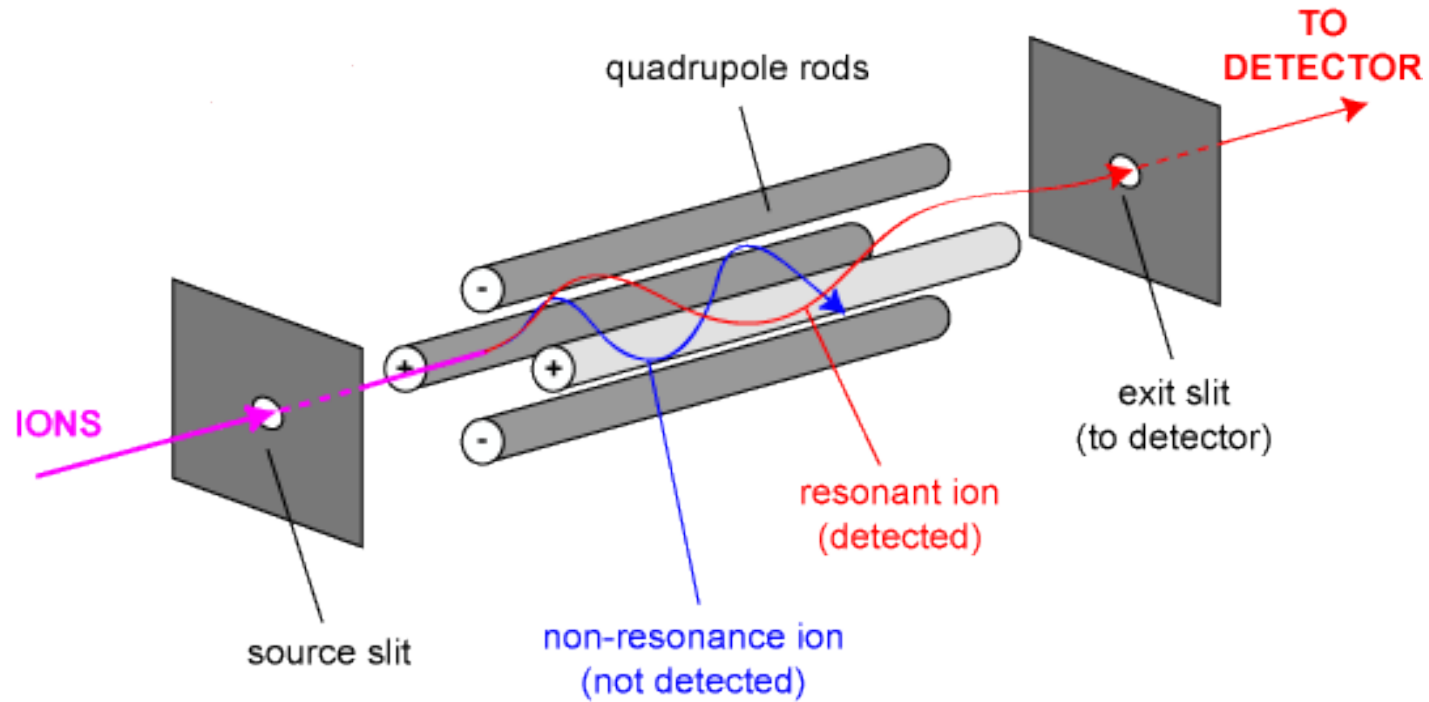
$$\overline{F} = \frac{mv^2}{R} = zvB$$

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



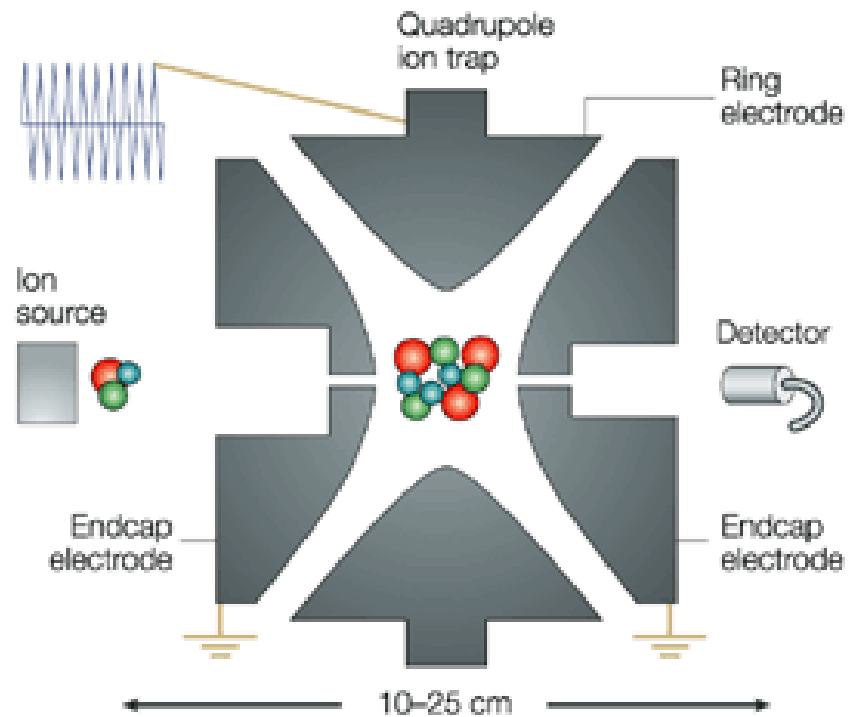
$$R = \sqrt{\frac{m}{z}} \sqrt{\frac{2V}{B}}$$

Quadrupole Mass Filter



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

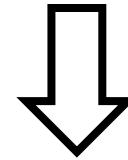
Ion Trap



Fourier transform ion cyclotron resonance



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



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

Orbitrap

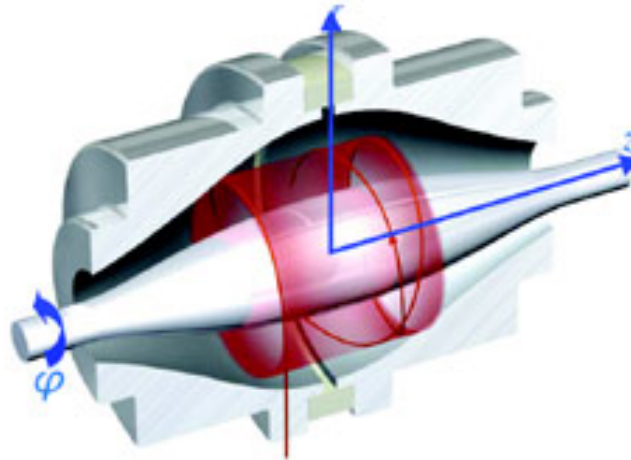
- Characteristic frequencies:

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

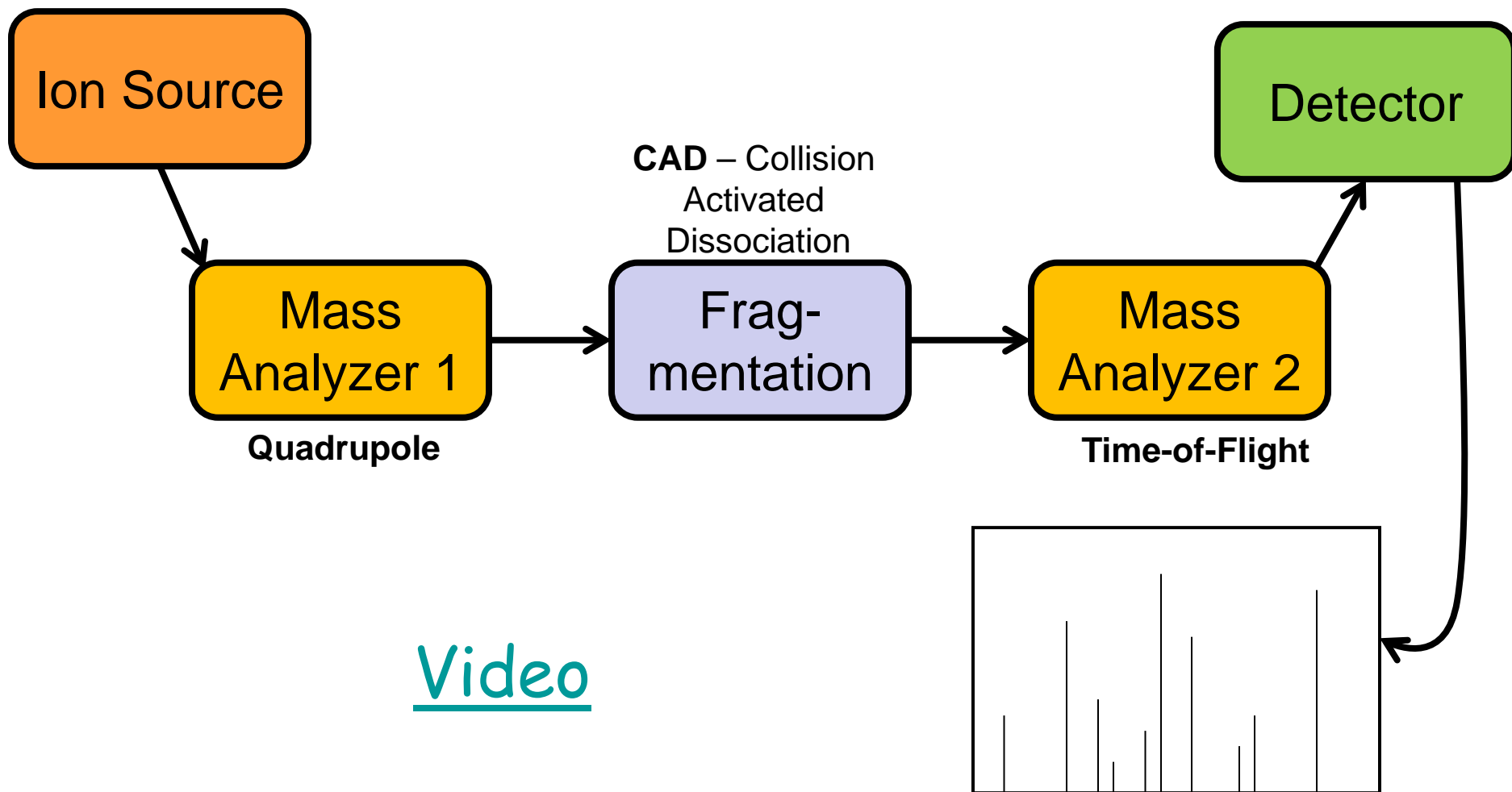
$$\omega_\varphi = \frac{\omega_z}{\sqrt{2}} \sqrt{\left(\frac{R_m}{R}\right)^2 - 1}$$

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

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

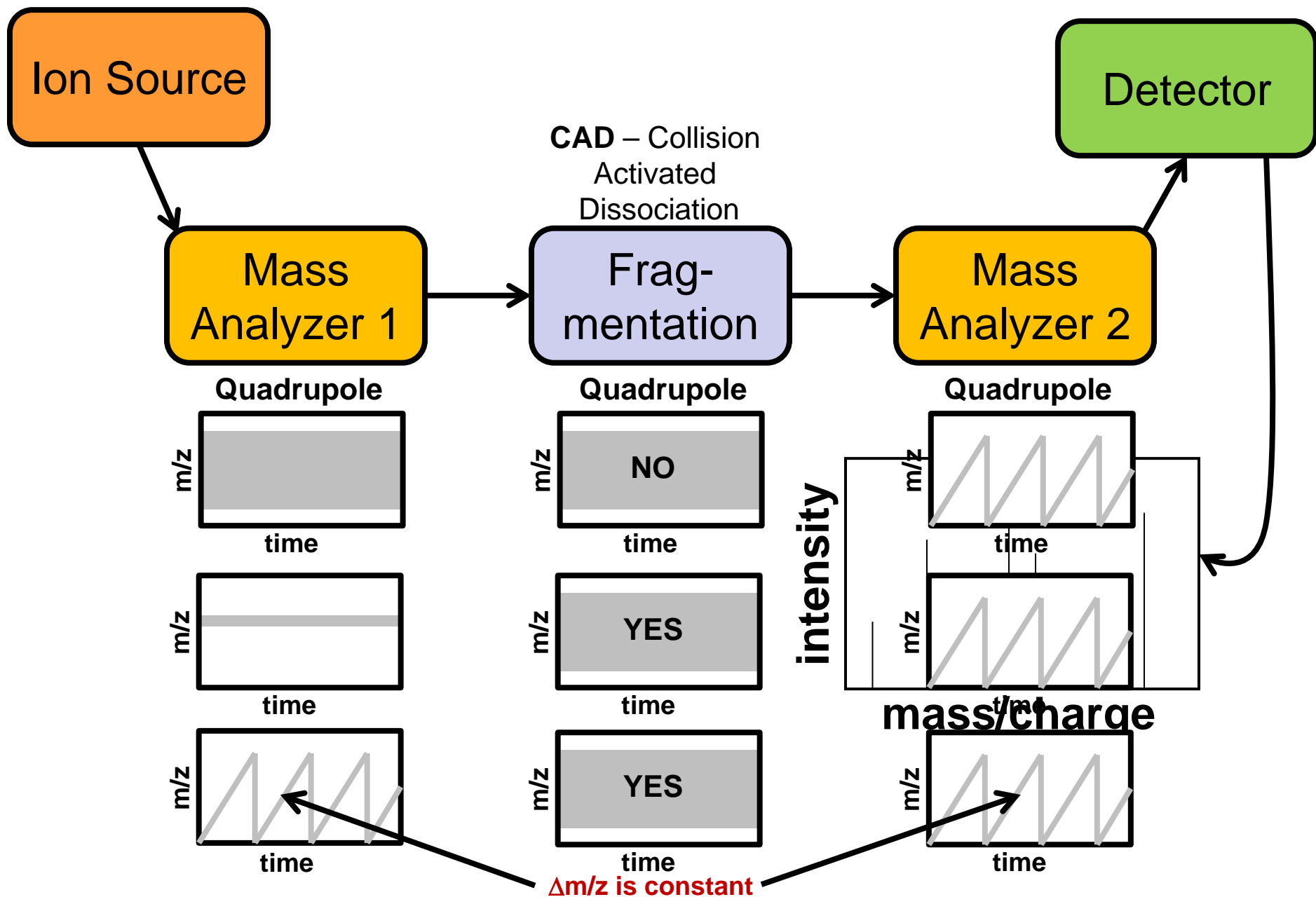


Quadrupole Time-of-Flight Mass Spectrometer

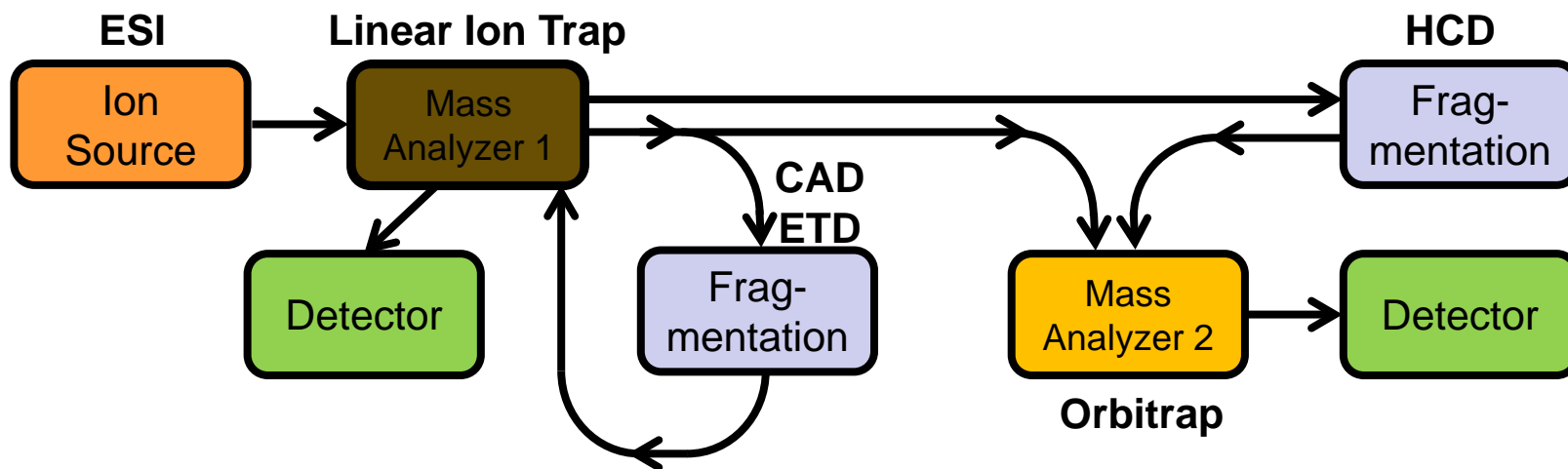


[Video](#)

Triple Quadrupole



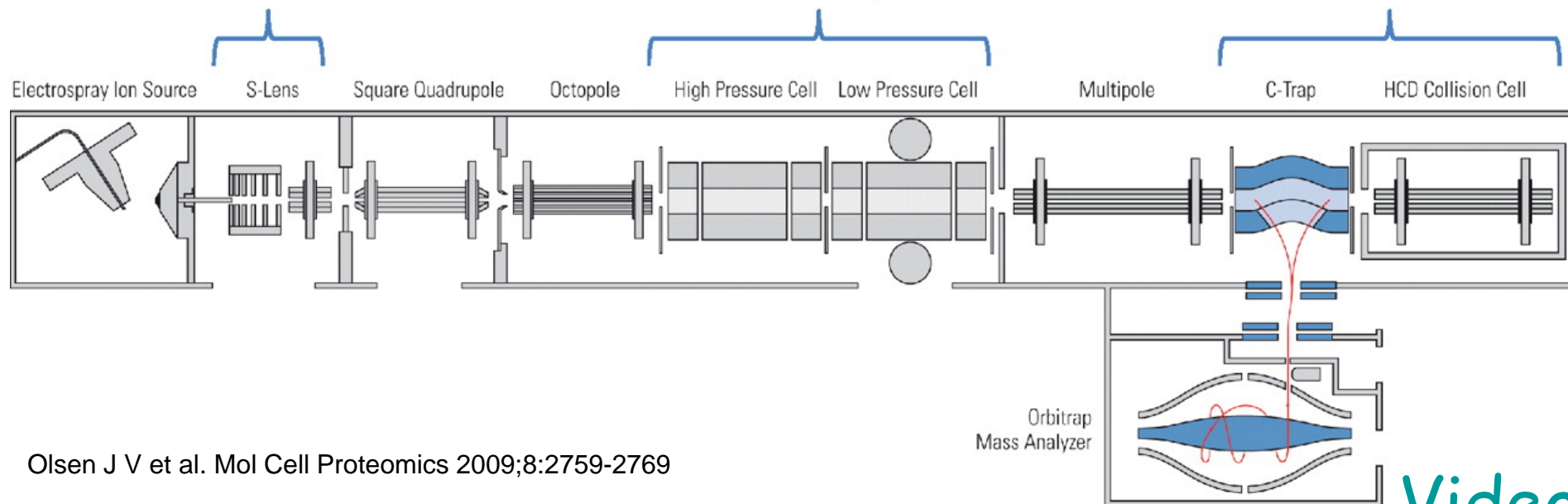
Linear Ion Trap / Orbitrap



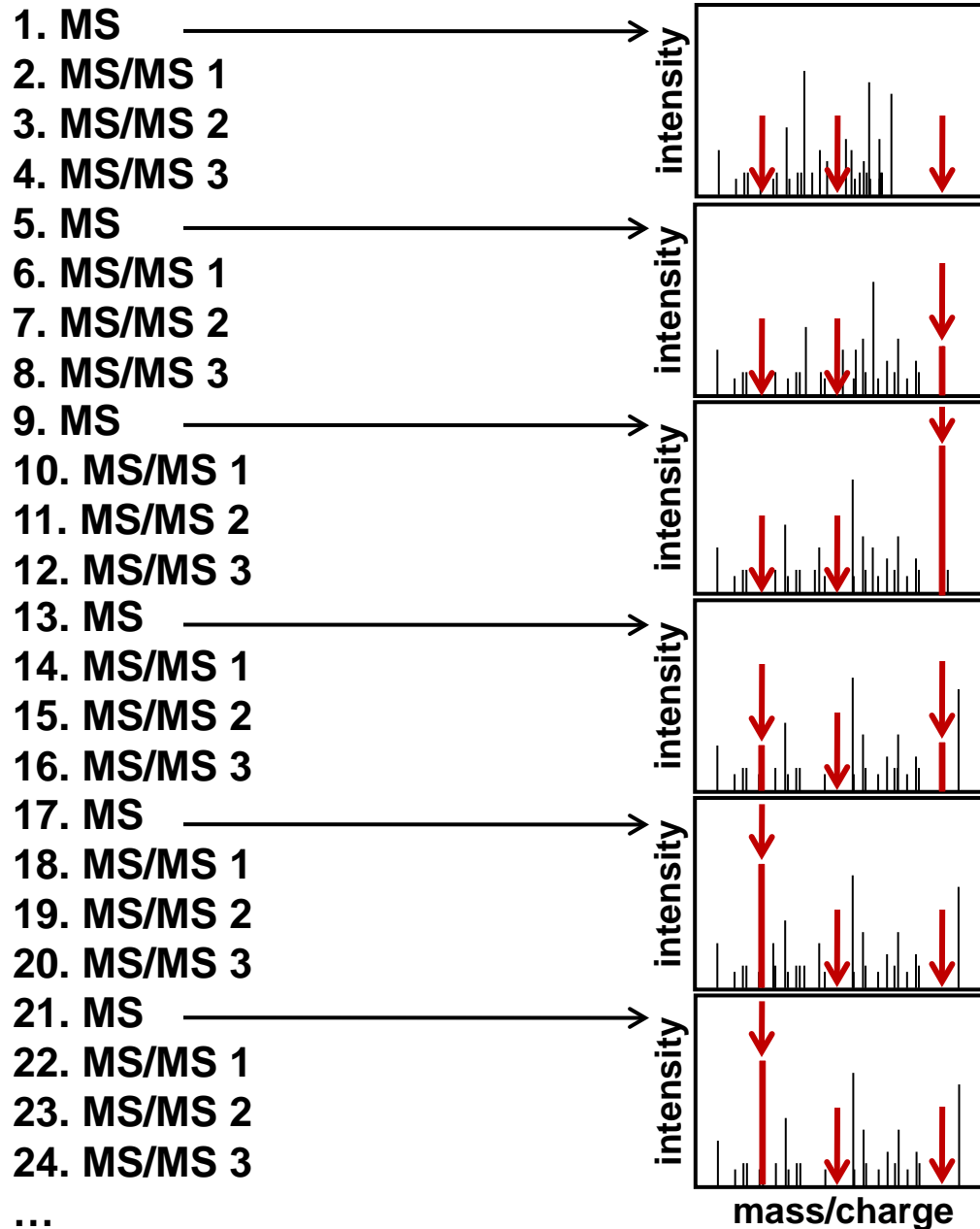
A. Stacked Ring Ion Guide

B. Dual linear ion trap

**C. Combo C-trap/
HCD collision cell**

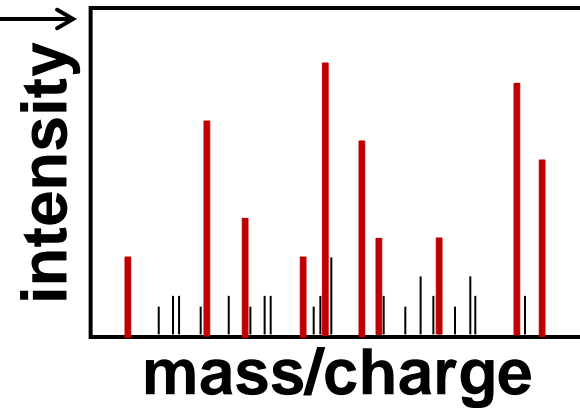


Data Independent Acquisition



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

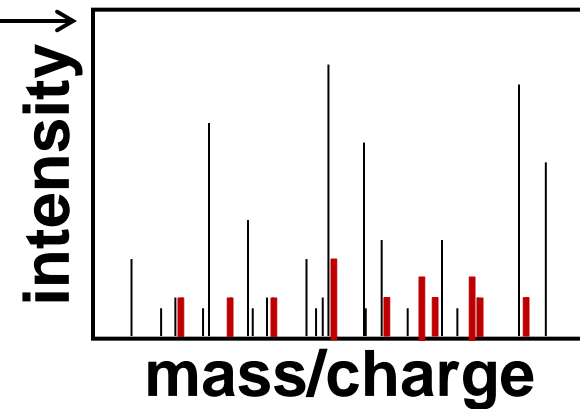
19. MS/MS 7

20. MS/MS 8

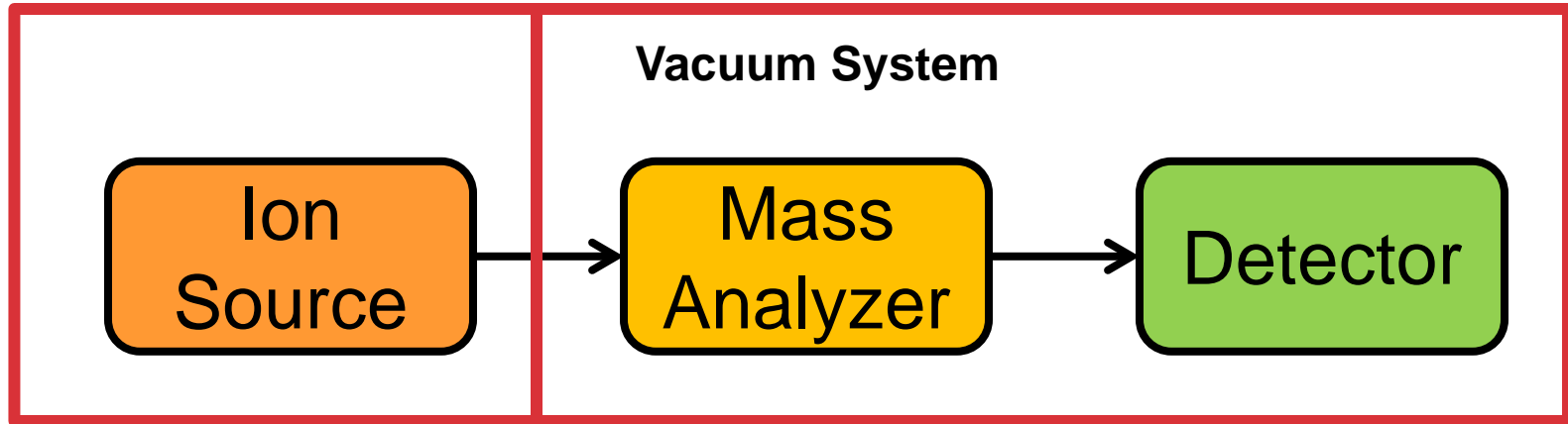
21. MS/MS 9

22. MS/MS 10

...



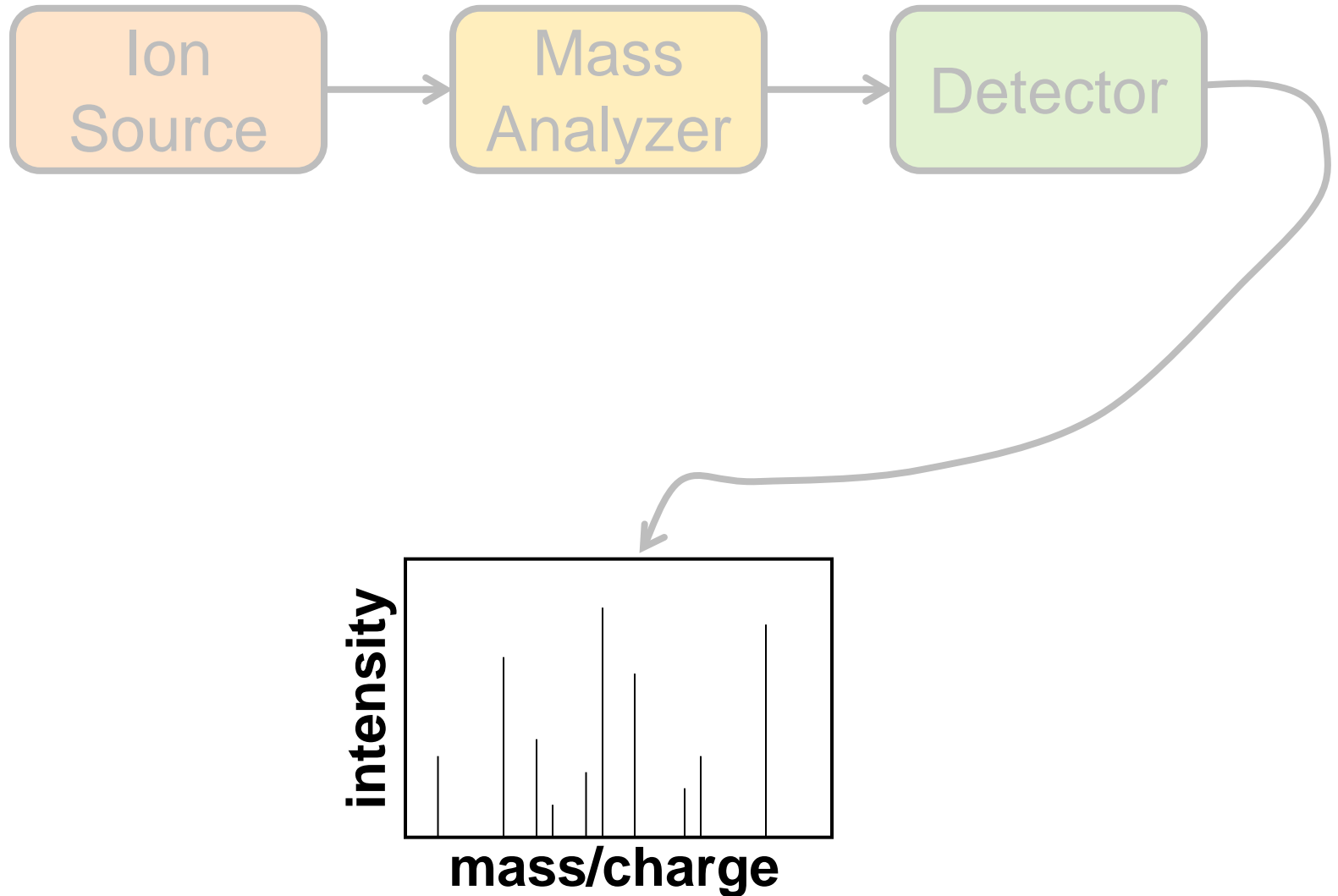
Vacuum System



Atmosphere



Mass Spectrometry Data



Mass Spectrometry Data

Dimensions:

Time

Peptide m/z

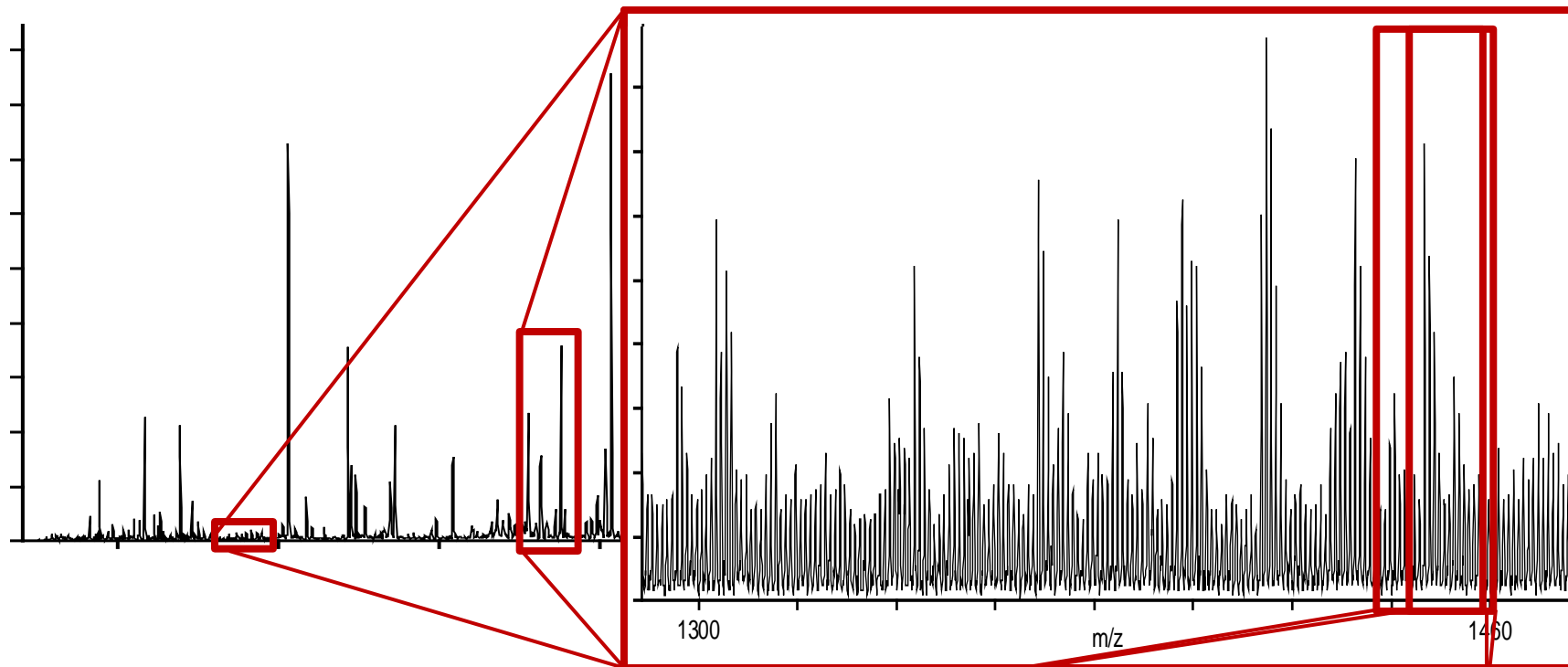
Peptide Intensity

Peptide fragment m/z

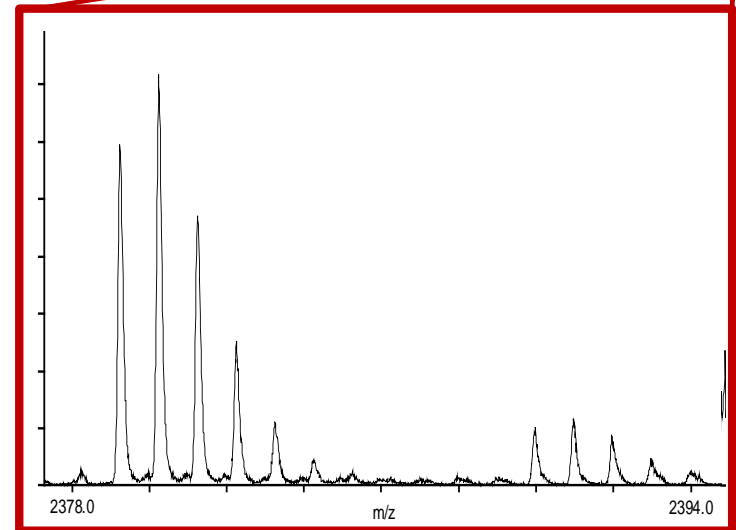
Peptide fragment intensity

...

Example data - MALDI-TOF

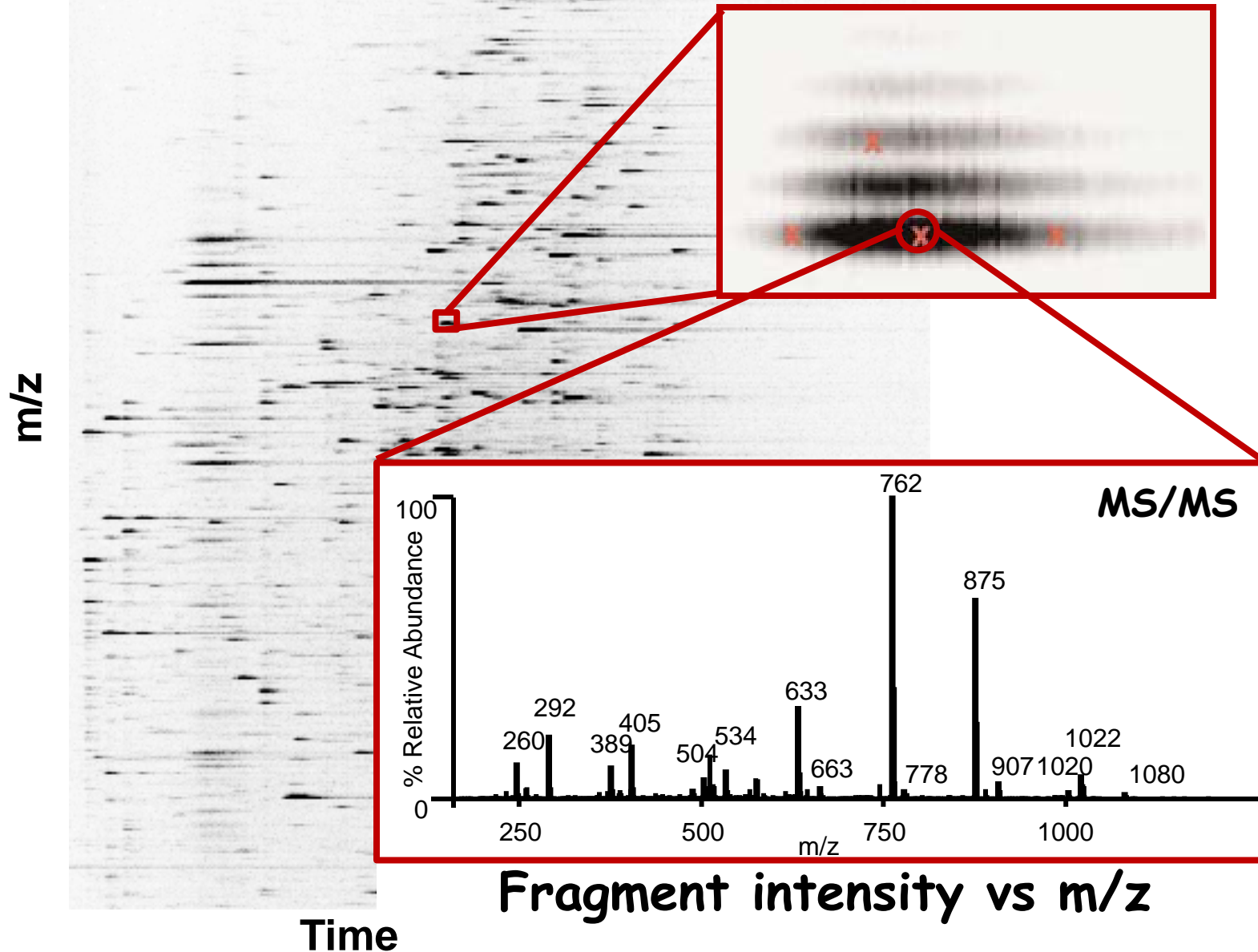


Peptide intensity vs m/z



Example data - ESI-LC-MS/MS

Peptide intensity vs m/z vs time

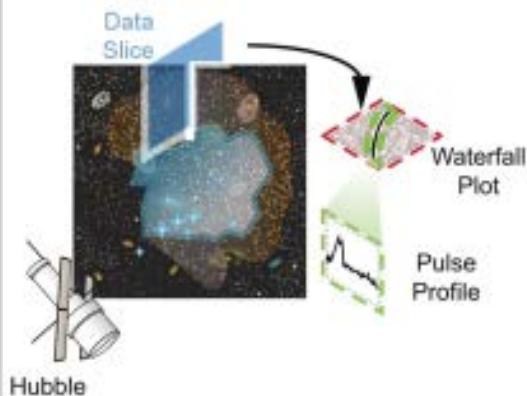


Slice - Scalable Data Sharing for Remote Mass Informatics

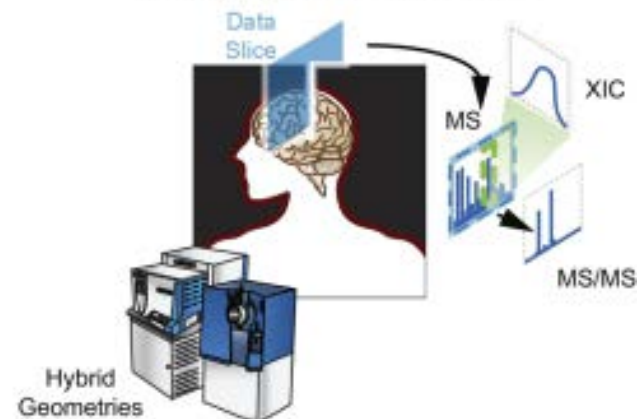


Developed by Manor Askenazi
slice.ionomix.com

Mapping Celestial Features

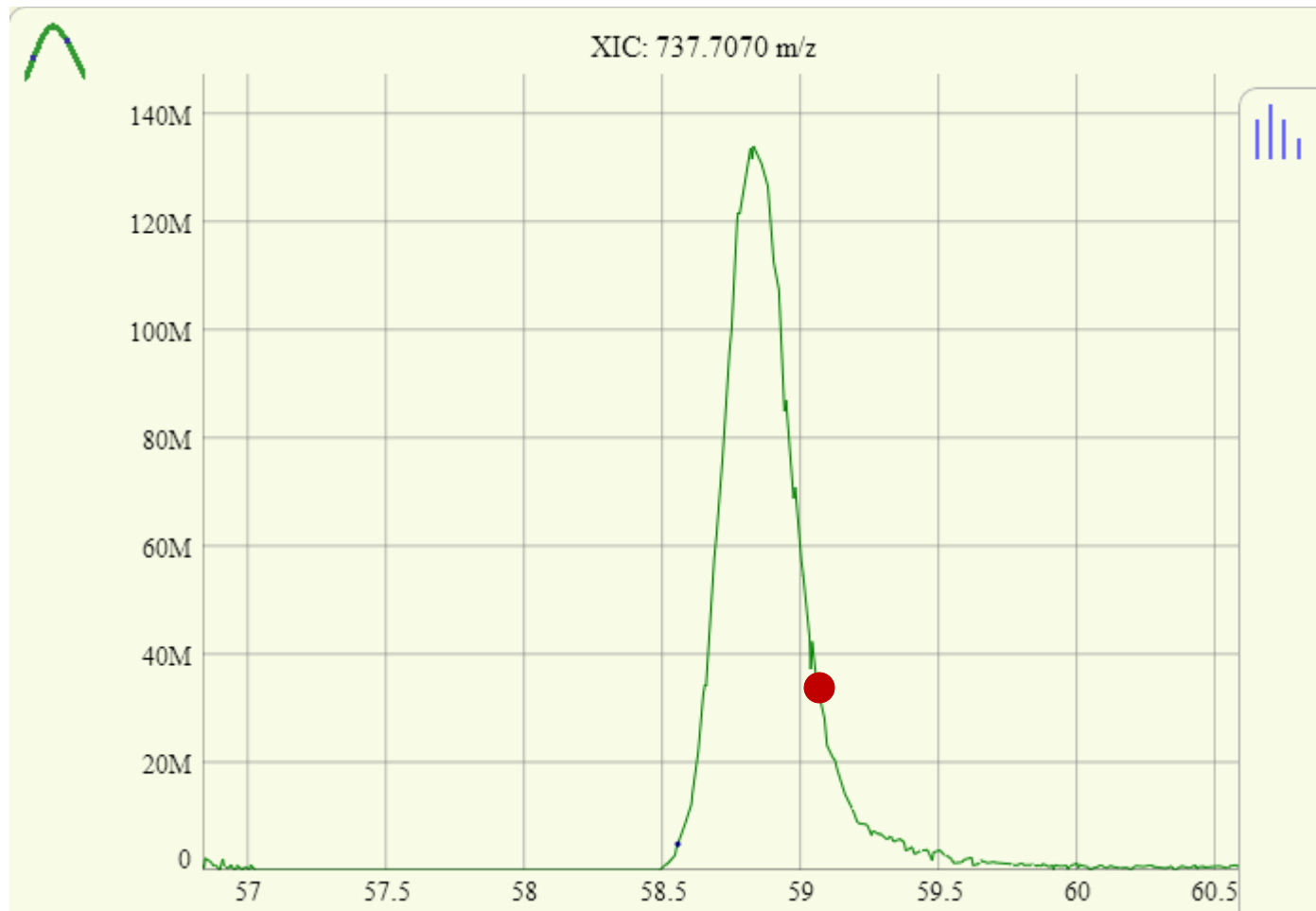


Mapping Human Proteins



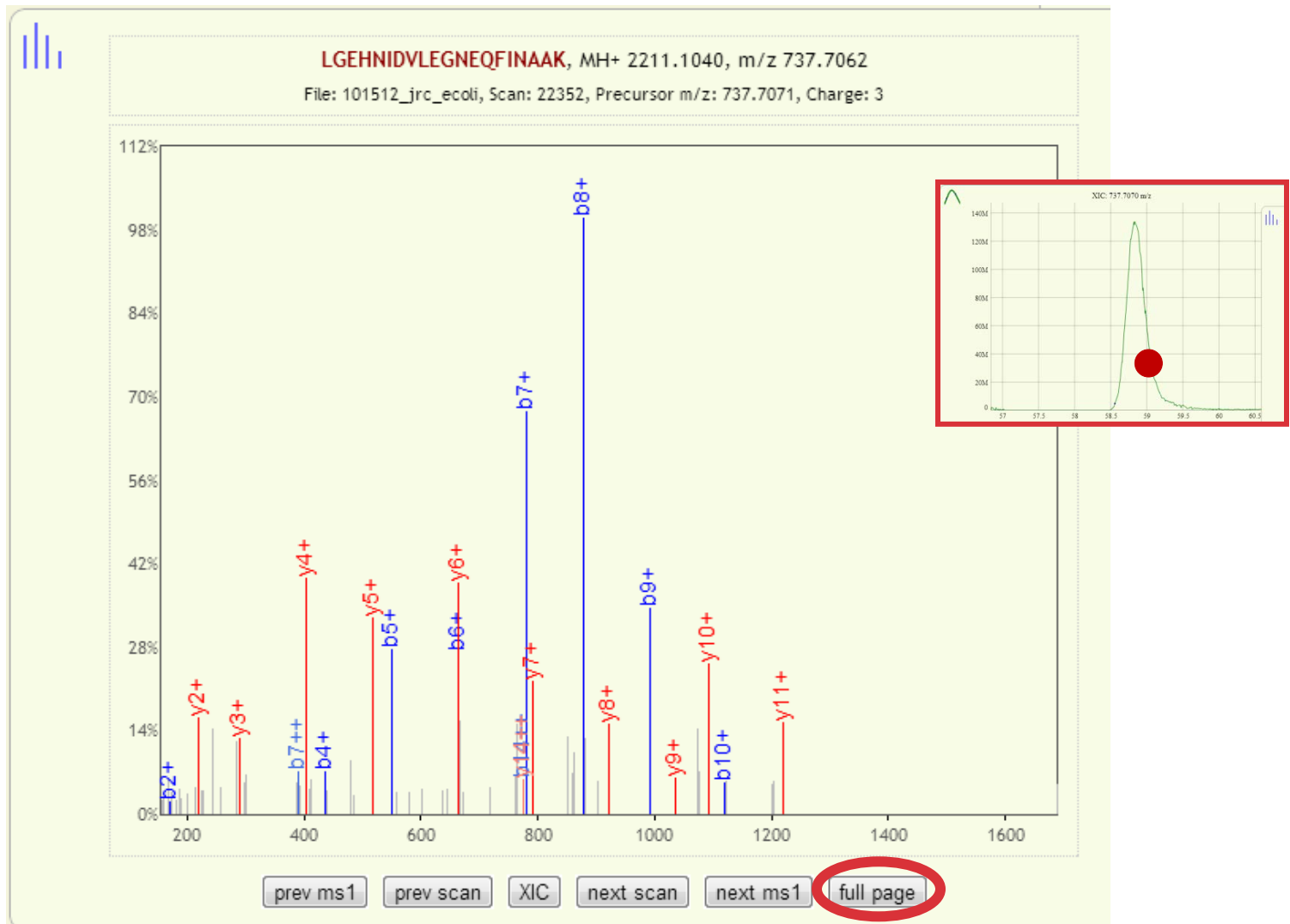
Most mass spectrometry data is acquired in discovery mode, meaning that the data is amenable to open-ended analysis as our understanding of the target biochemistry increases. In this sense, mass spectrometry based discovery work is more akin to an astronomical survey, where the full list of object-types 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



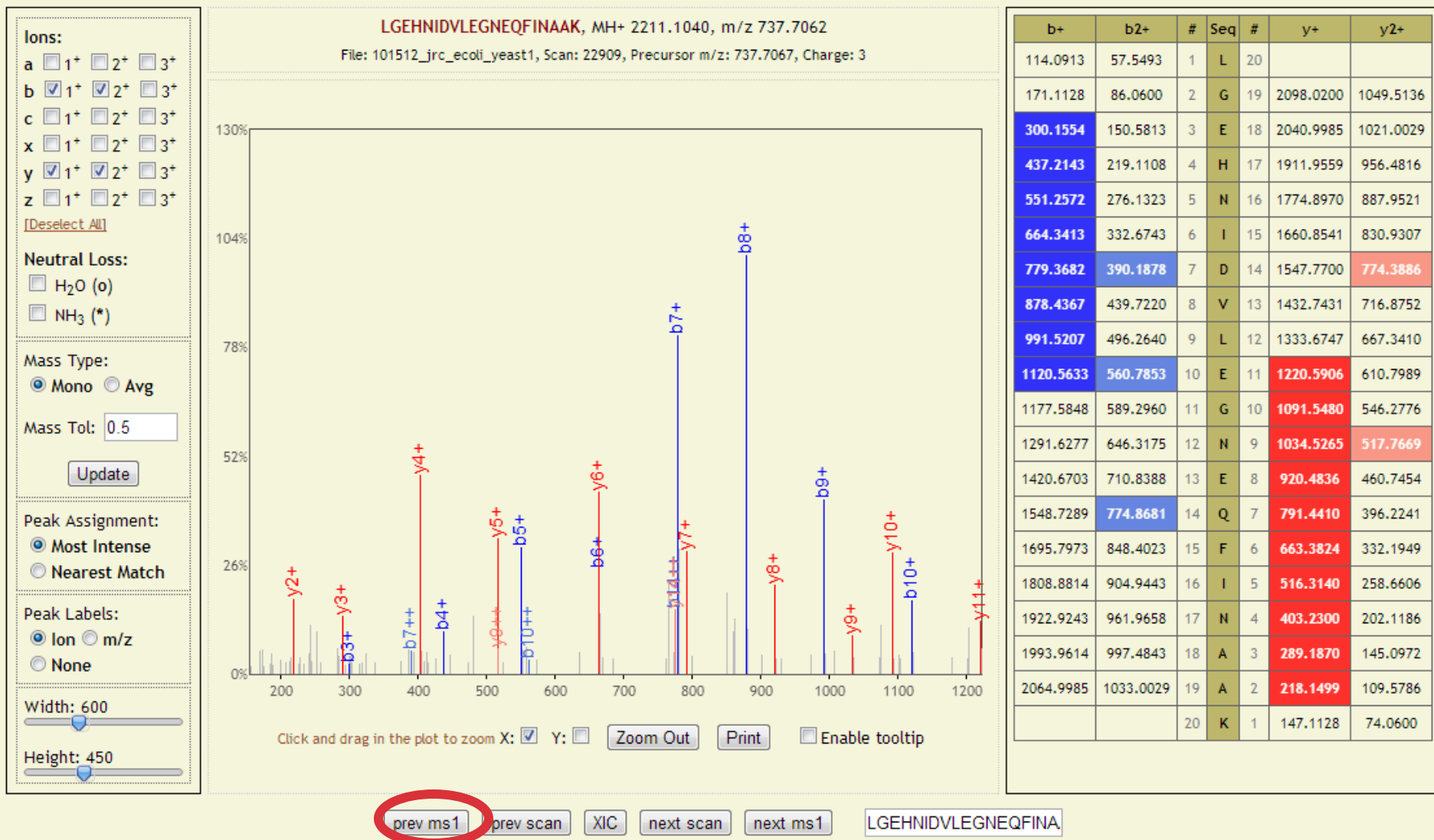
Peptide intensity vs time
For 737.707 m/z which corresponds to
3+ of LGEHNIDVLEGNEQFINAAK

Example Mass Spectrometry Data



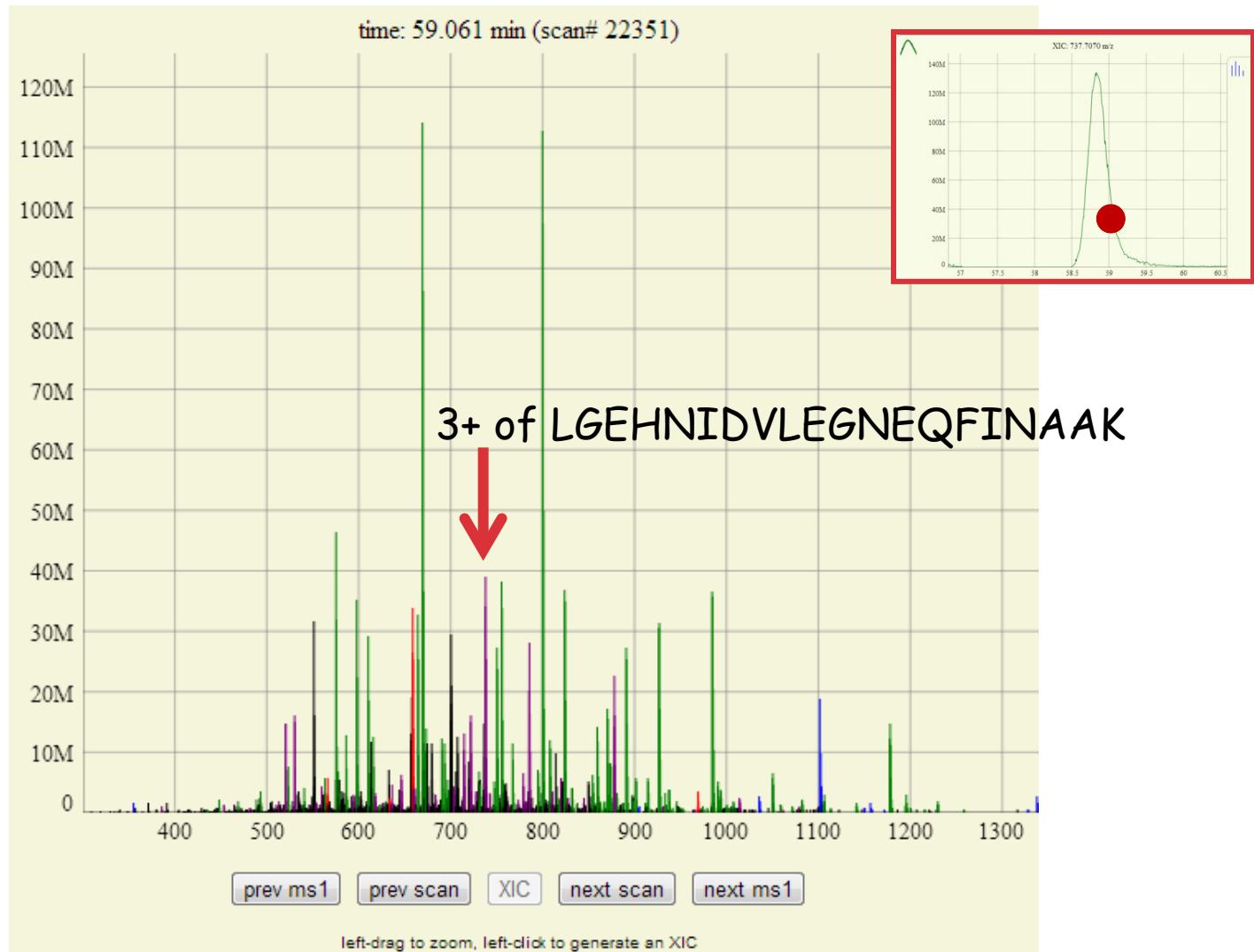
Fragment intensity vs m/z
For 3+ of LGEHNIDVLEGNEQFINAAK

Example Mass Spectrometry Data



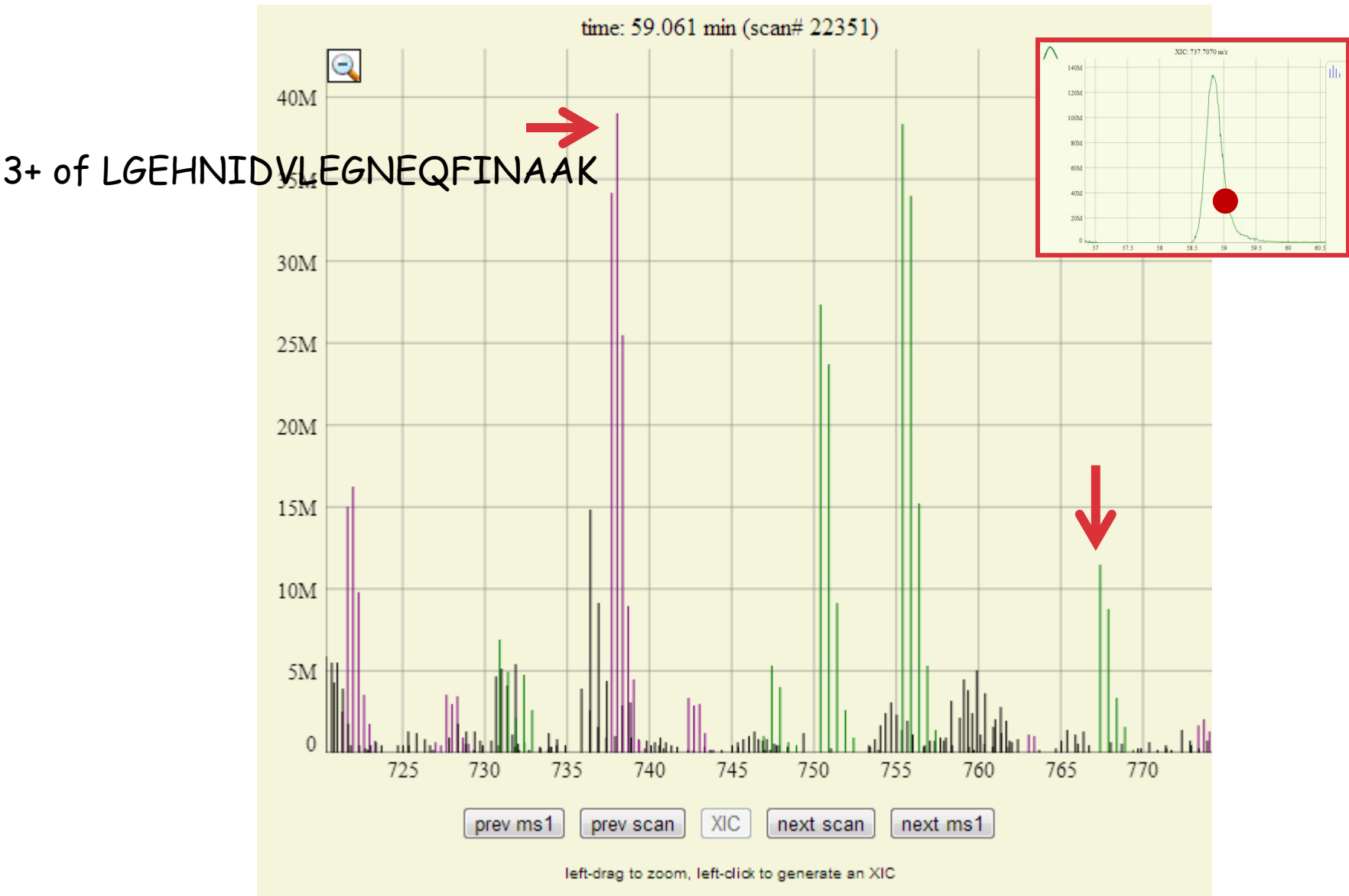
Fragment intensity vs m/z
For 3+ of LGEHNIDVLEGNEQFINAAK

Example Mass Spectrometry Data



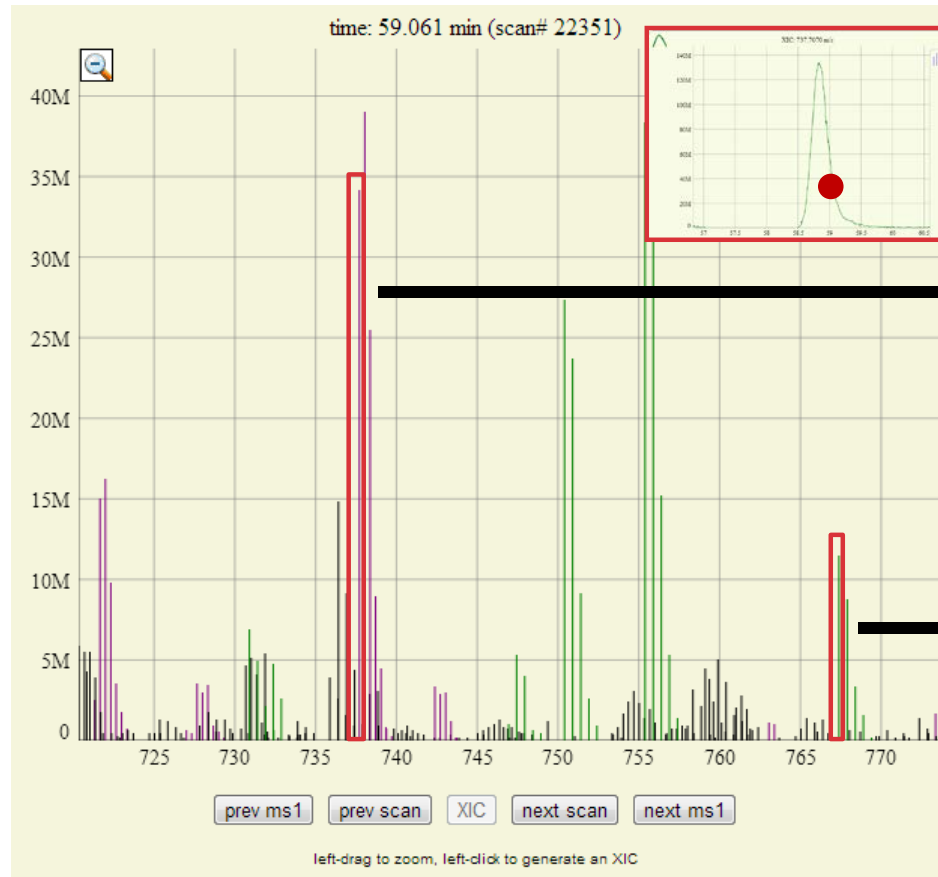
Peptide intensity vs m/z

Example Mass Spectrometry Data

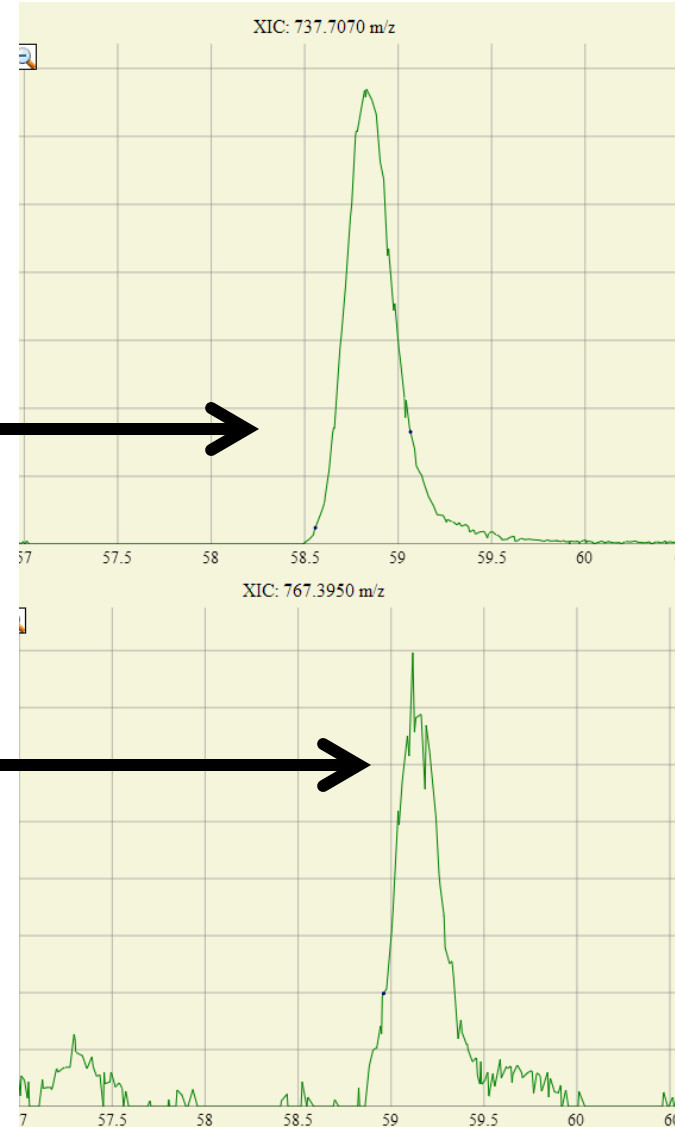


Peptide intensity vs m/z

Example Mass Spectrometry Data



Peptide intensity vs m/z



Peptide intensity vs time

OpenSlice Data Sharing Platform

Overview

Research

Members

Publications

Presentations

Tools

Contact

Center for Health
Informatics and
Bioinformatics



OpenSlice is a novel web-based API for large scale data sharing in Mass Spectrometry *fully eliminating the need to download RAW datafiles*. More documentation will be made available soon, however for the time being, a slightly outdated **ASMS2013 talk** is available, as well as 4 example D.I.C.E (Distribute Ion Chromatogram Extractor) viewers for the CPTAC Colon Dataset:

- **Ascending Colon:** full interactive access to **190 Rawfiles** from 12 patients having a tumor in the ascending colon. Data are colored by history of polyps.
- **Lymphatic Invasion:** full interactive access to **660 Rawfiles** from 44 patients with lymphatic invasion. Data are colored by disease stage.
- **Duplicate:** Technical replicates of a patient dataset consisting of **30 Rawfiles** (duplicates of 15 fractions). Data are colored by replicate date.
- **Complete:** full interactive access to **1402 Rawfiles** from 90 patients with Colon cancer. Data are colored by Gender. *Note: This will break your browser!!!*

Currently, only **Chrome** is recommended for the interactive, browser-based slicing and dicing of these datasets.

Openslice.fenyolab.org

Proteomics Informatics - Overview of Mass spectrometry (Week 2)

