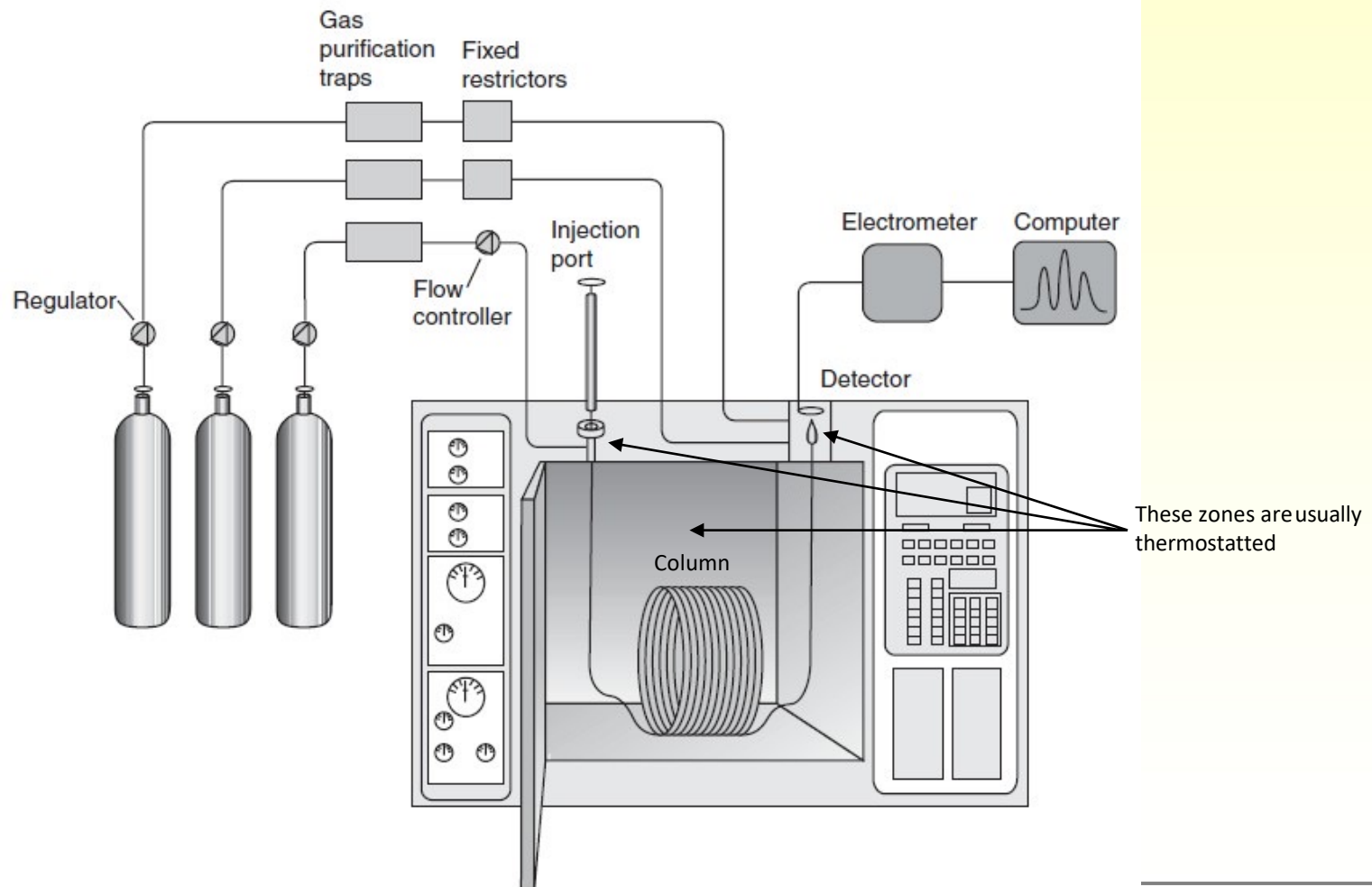
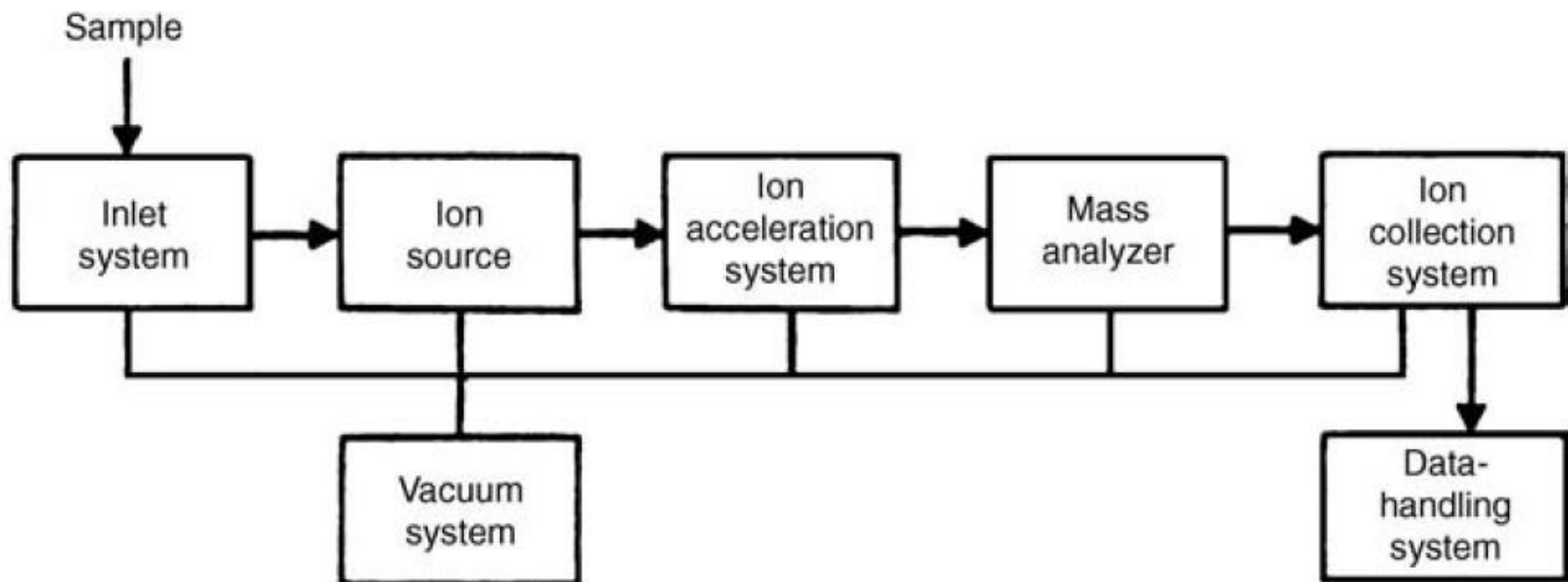


Gas and liquid chromatography with mass spectrometric detection

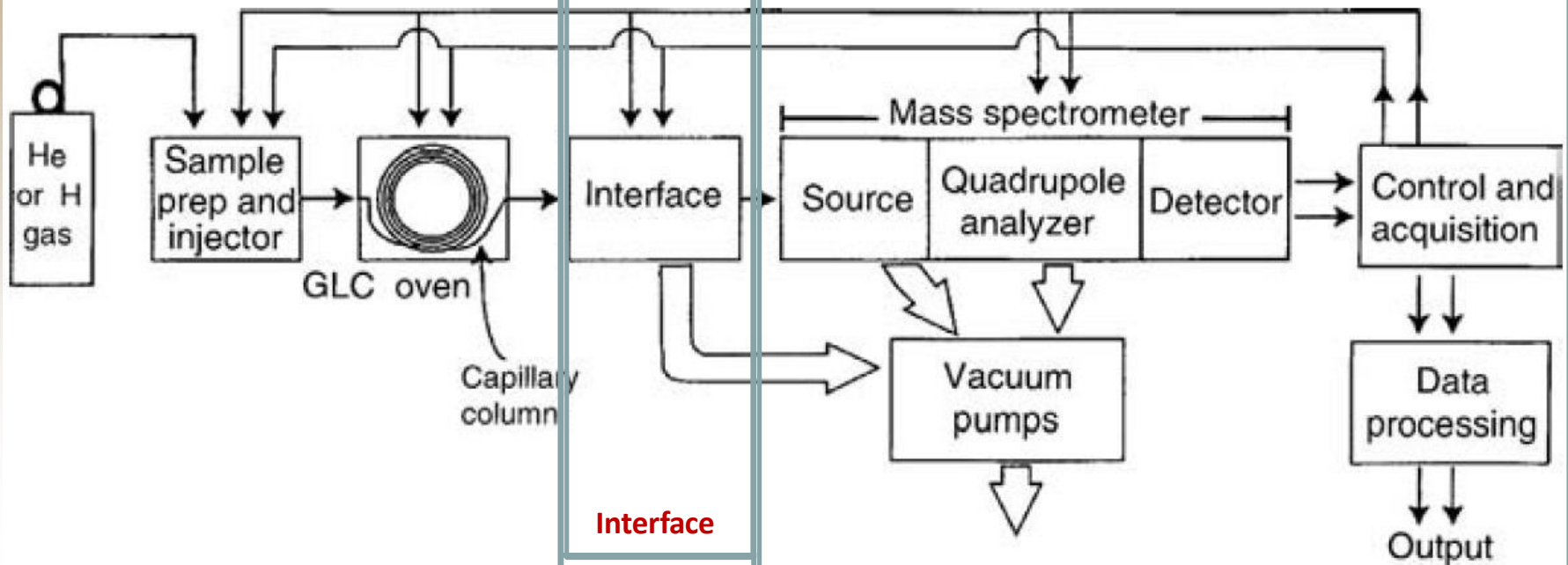
Gas chromatograph



Mass spectrometer



Parts of GC-MS system



Gas chromatograph

Mass spectrometer

GC-MS animation



Gas Chromatography- Mass Spectrometry

Key method features

Simultaneous **Separation + Identification**

Huge amount of information about the sample in single run

Very high selectivity in selected ion monitoring mode (SIM)

Multi-analyte selective and sensitive method can be developed

Ionization Methods

Gas Phase Ionization (mainly for volatile compounds)

Electron impact

Chemical ionization

Ionization in electric field

Liquid Phase Ionization (for large soluble molecules)

Electrospray

Atmospheric pressure chemical ionization (APCI)

Inductively coupled plasma

Ionization Methods

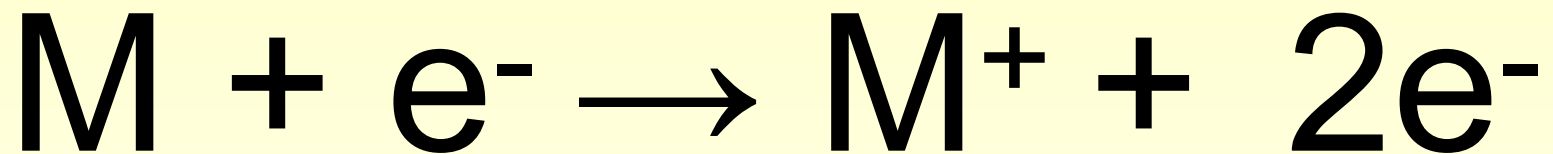
Solid Phase Ionization (for solid matrices)

Laser ablation

Fast atoms bombardment

Matrix-assisted laser desorption/ionization (MALDI)

Electron impact ionization



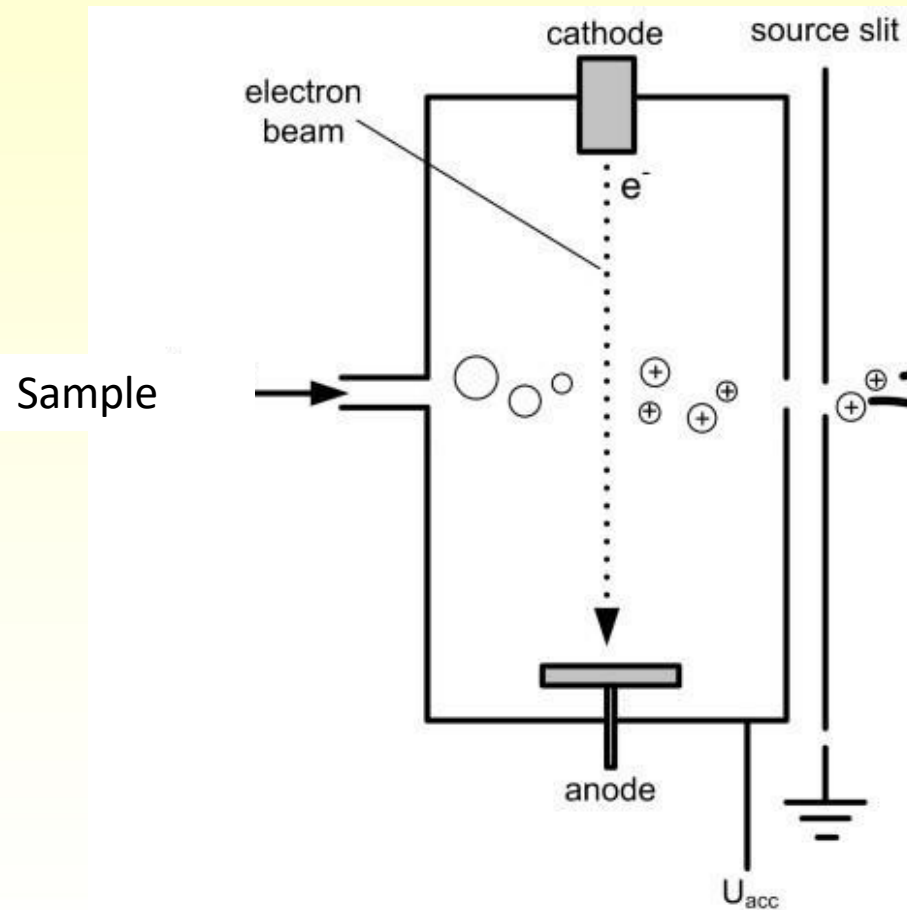
Mostly used method for ionization of organic molecules

Ionization energy is usually equal to 70 eV that corresponds to a length of typical chemical bond in organic molecules

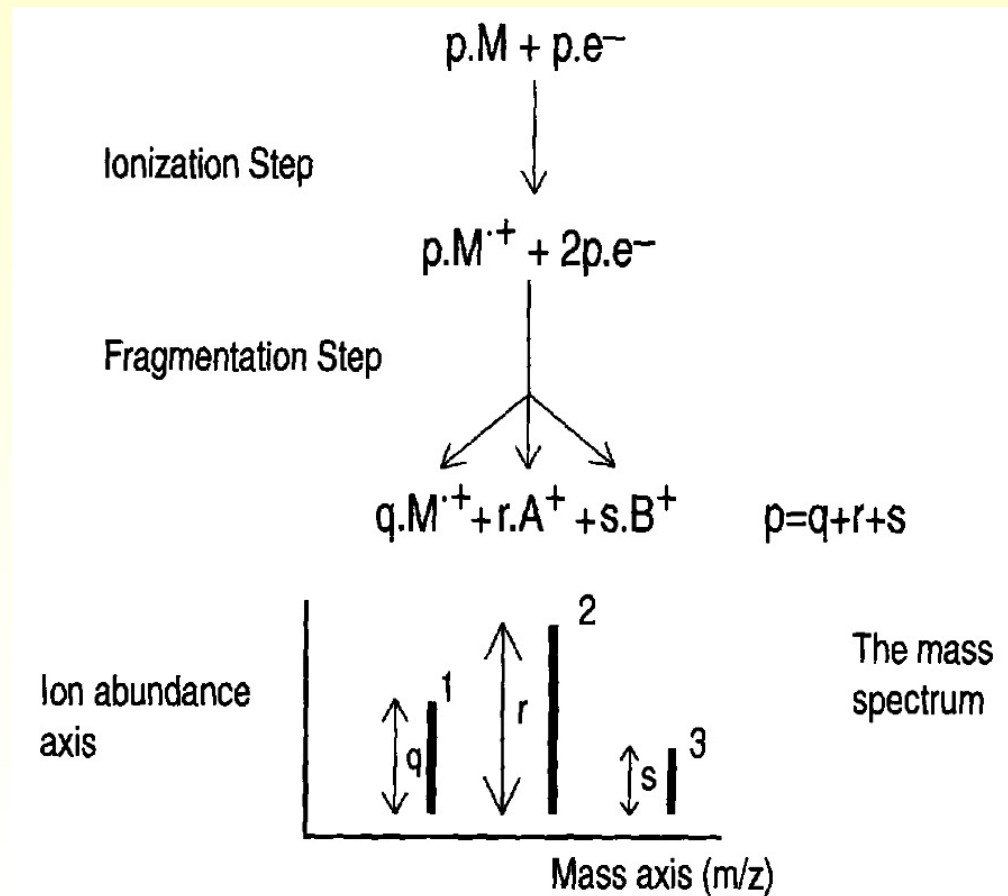
Ionization is held in vacuum to avoid formation of ions of atmospheric gases capable to recombine with analyte ions and degrade them

Allows collecting mass spectra containing structural information that can be used for reliable identification of molecules

Electron impact ionization (scheme)

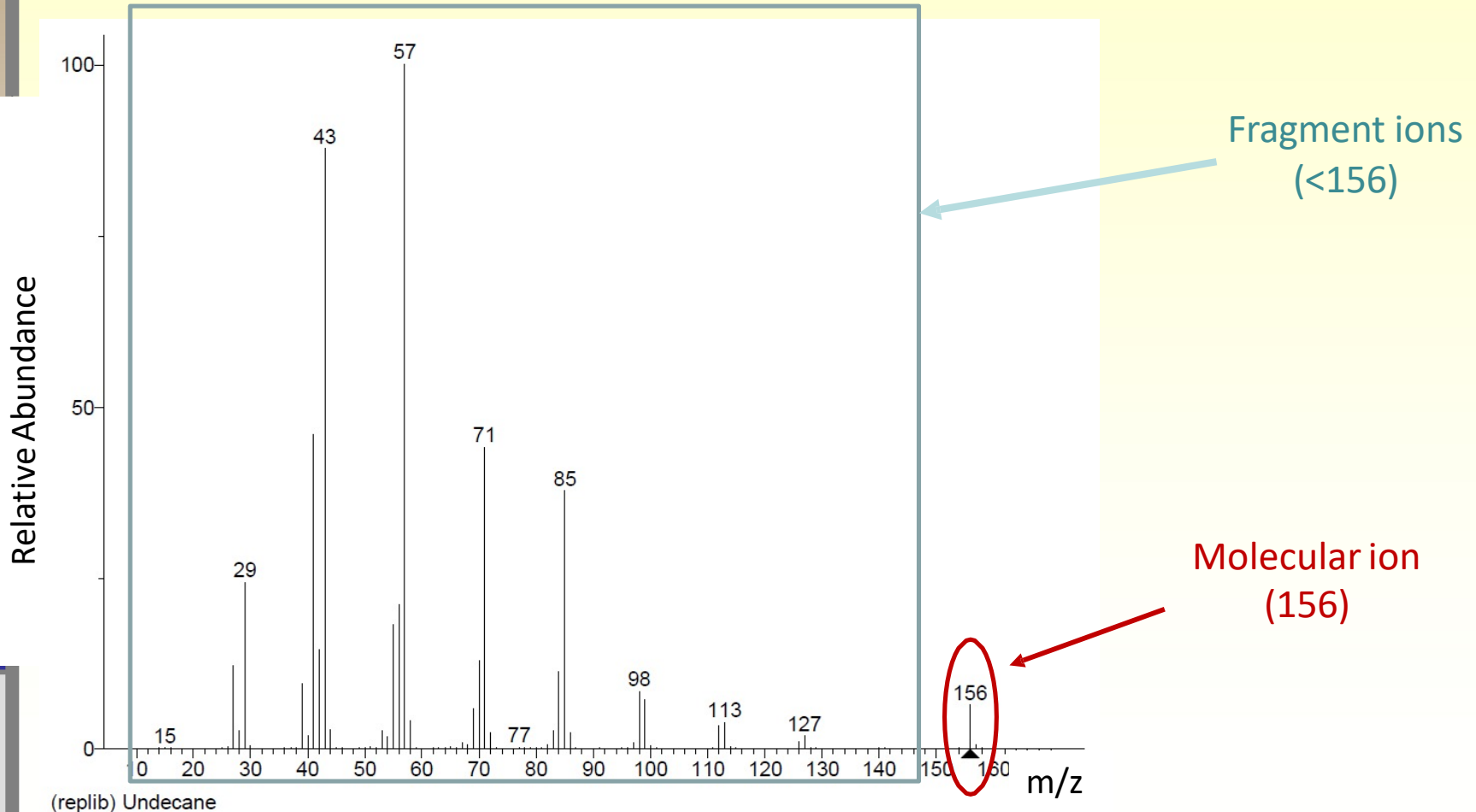


Electron impact ionization

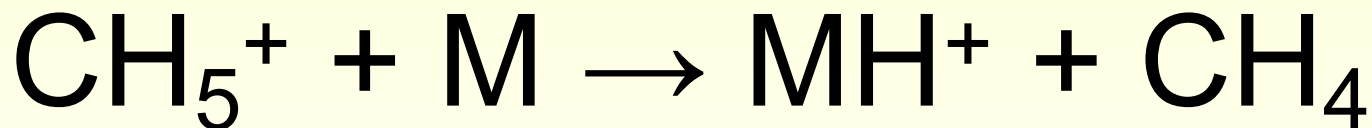
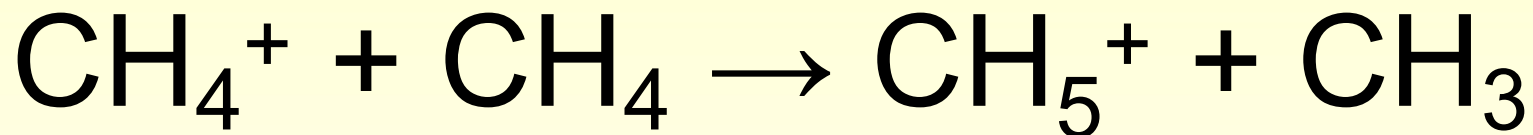
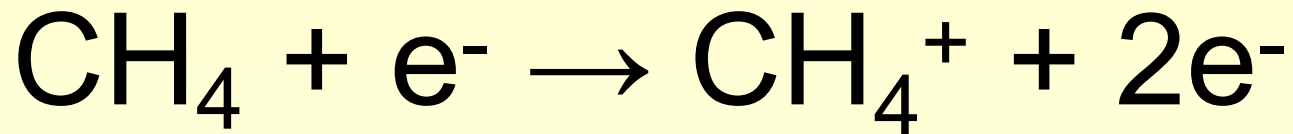


Mass spectrum (EI)

MS shows how many ions of each m/z were formed during ionization



Chemical ionization



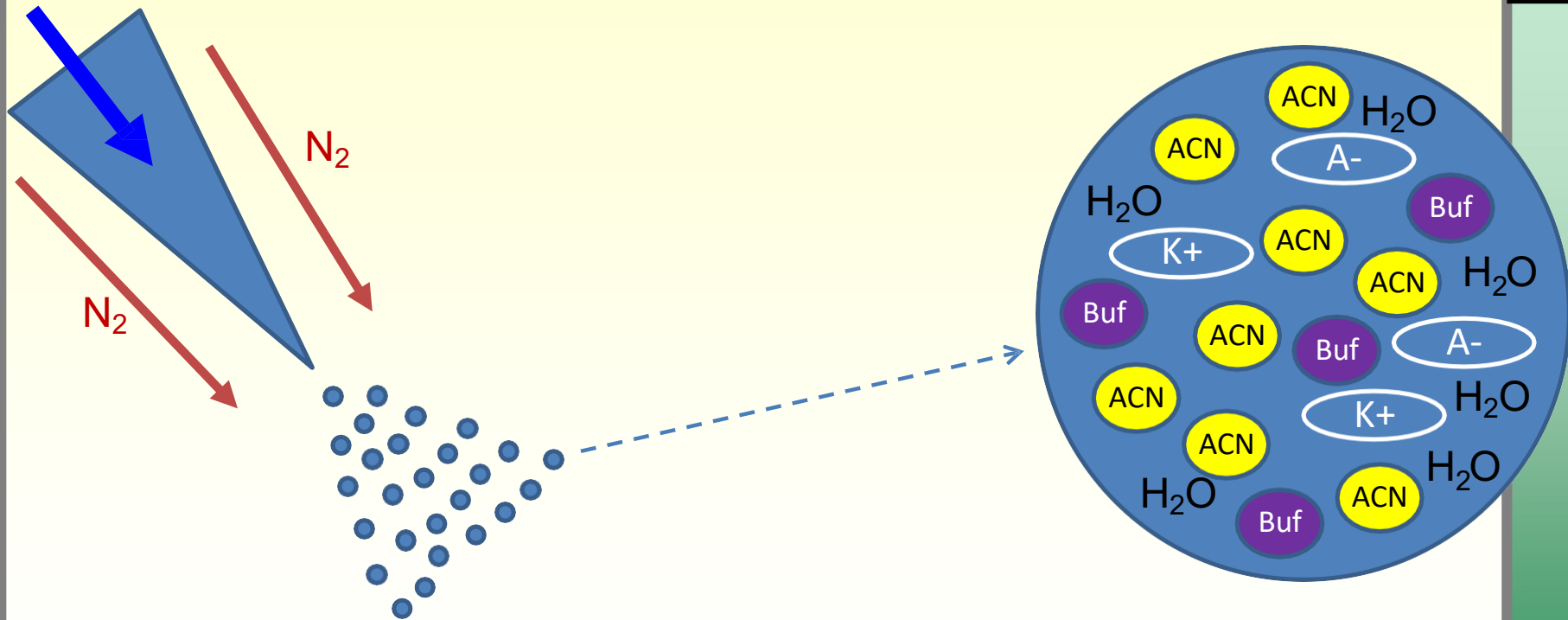
This soft ionization technique allows obtaining of intensive molecular ion

In most cases provides higher sensitivity of determination compared to EI

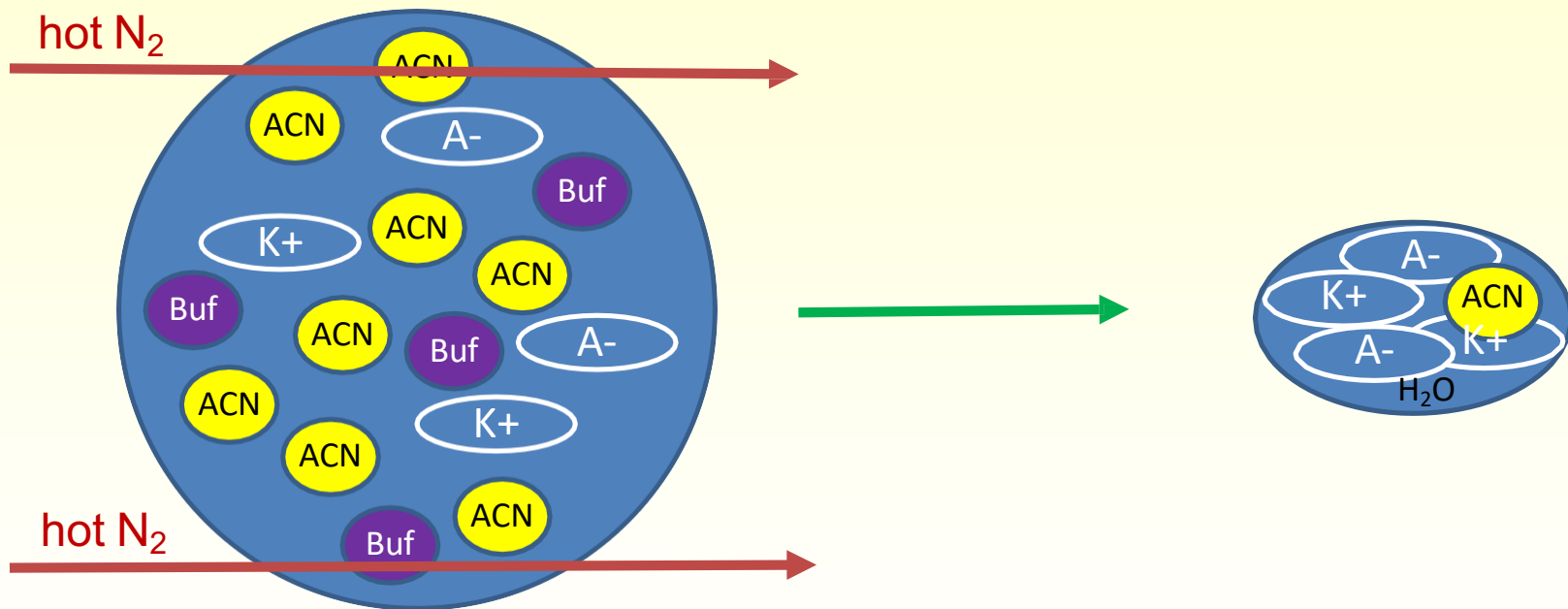
Method is perfect for analysis of non-stable compounds and molecules that can not be efficiently ionized by EI ionization

Electrospray ionization

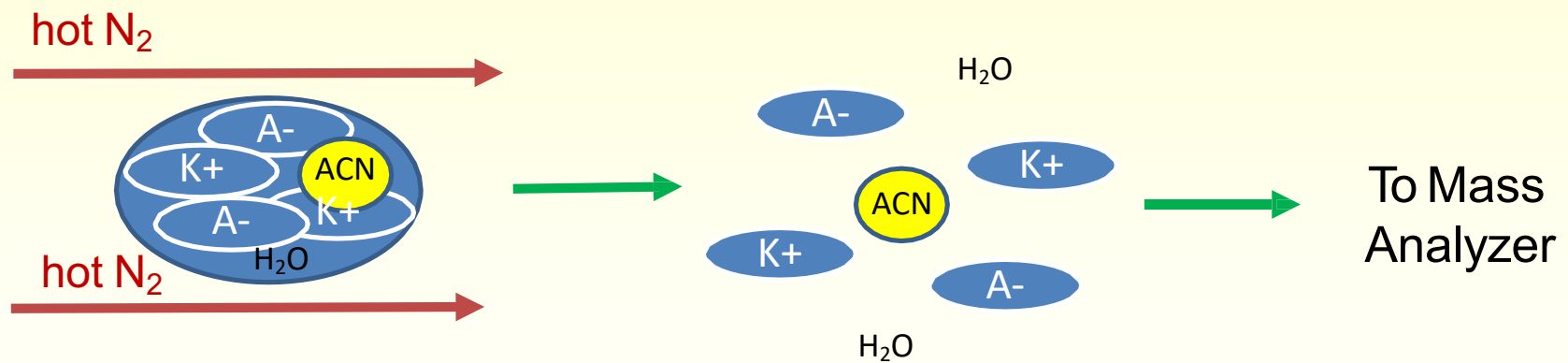
Flow from
LC column



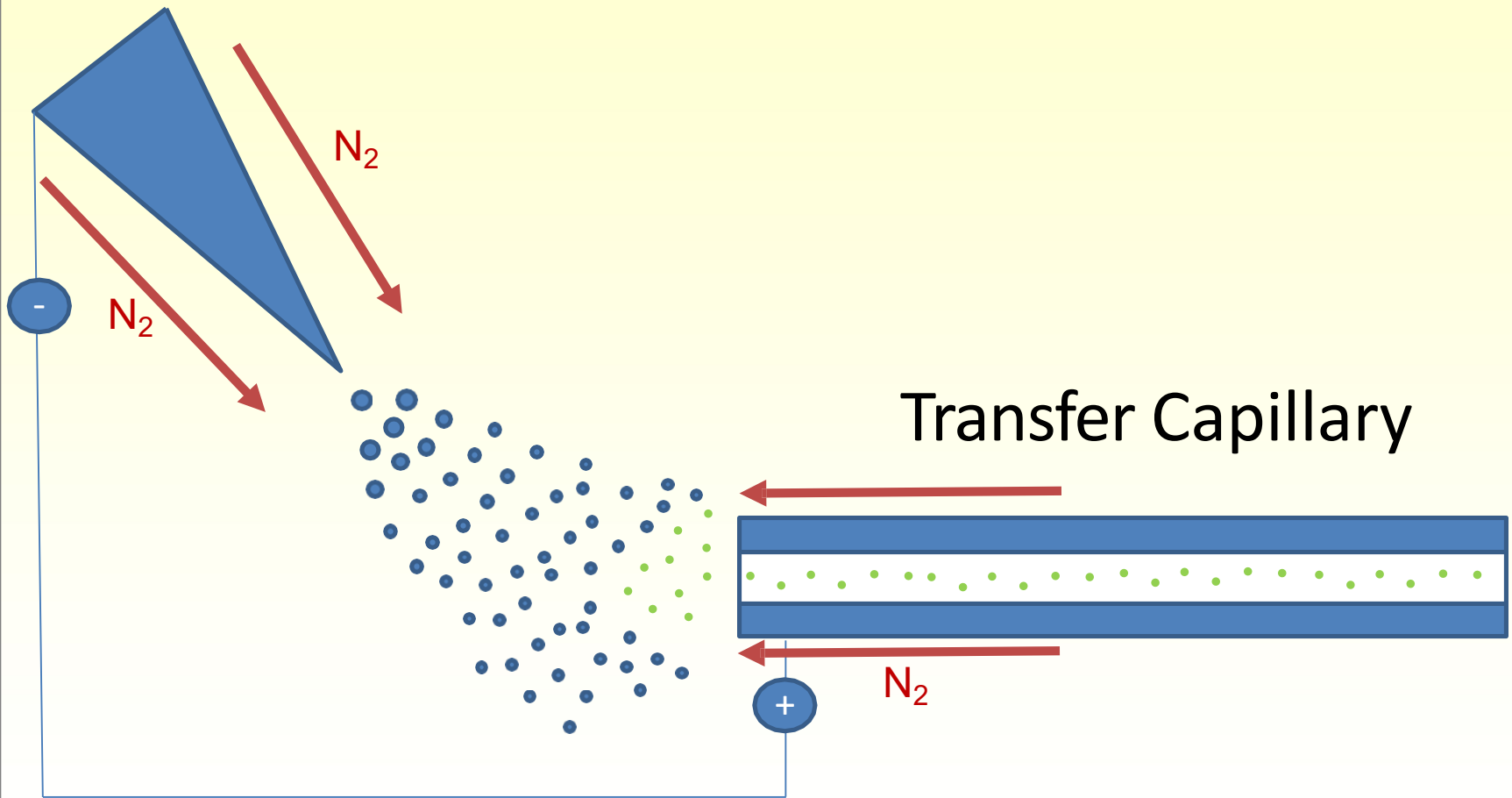
Mobile phase removal



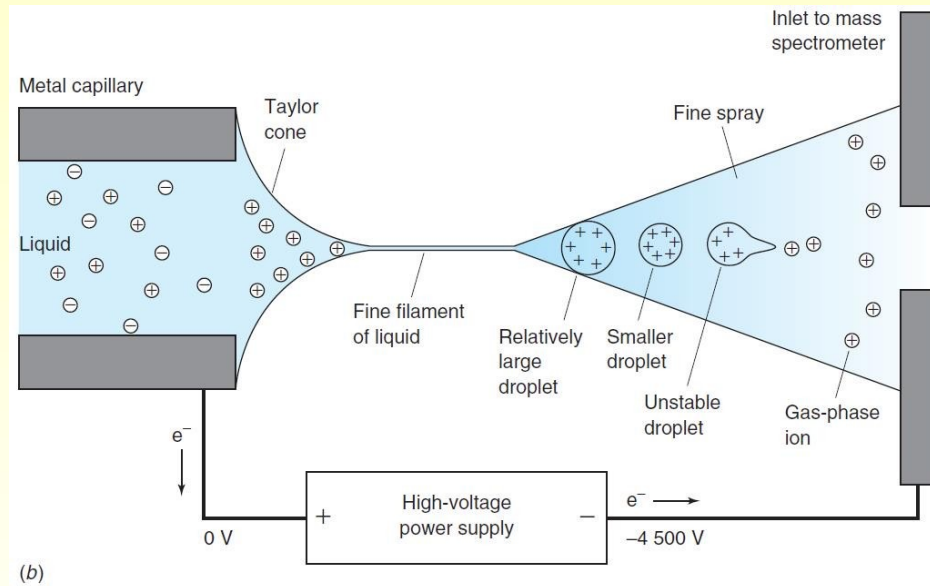
Explosion



Electrospray ionization



Electrospray ionization



Identification of analytes (EI)

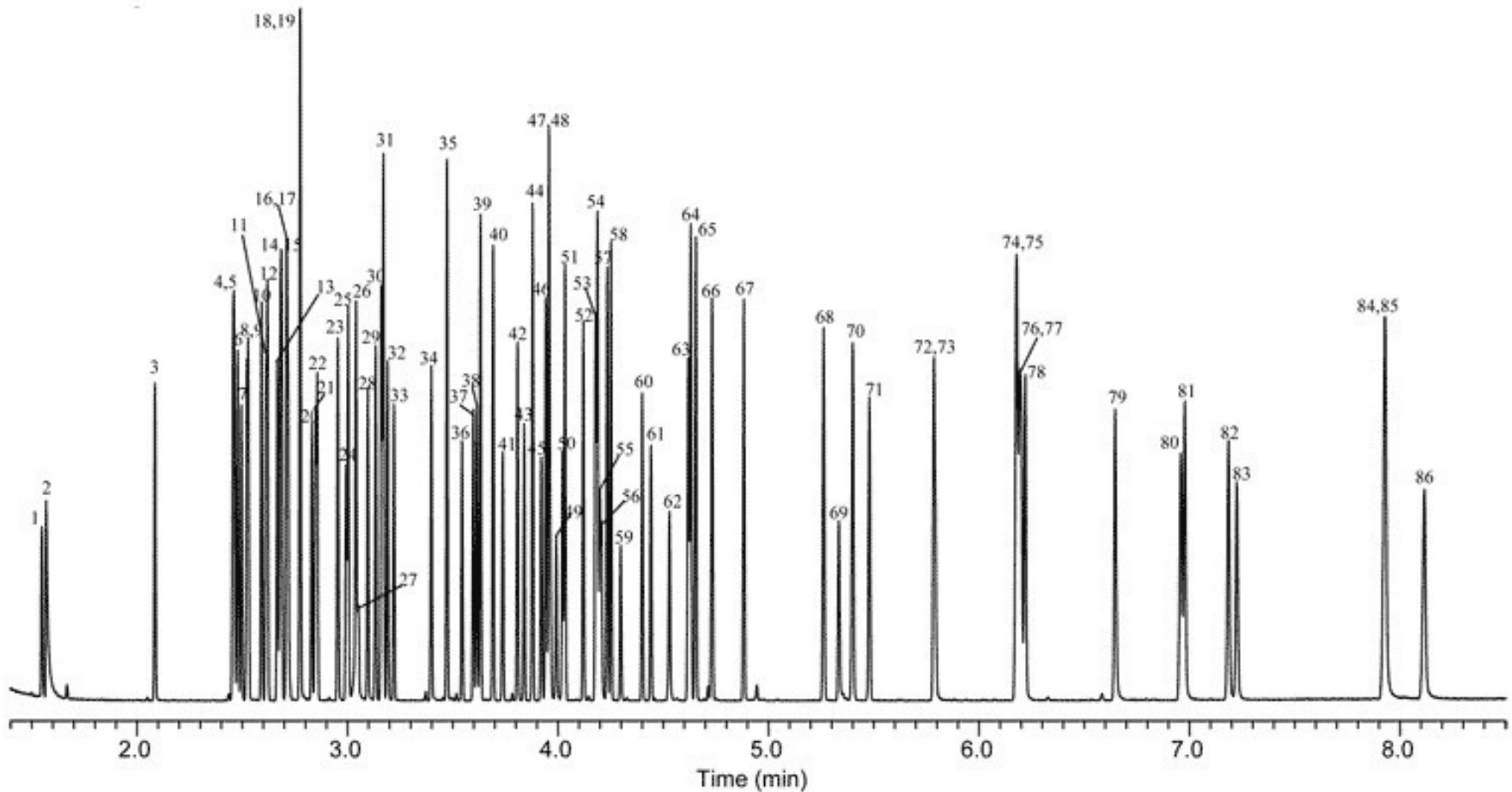
Full mass spectrum is collected in every point of total ion chromatogram (TIC)

Very pure spectra of compounds are obtained due to pre- separation of analytes > reliable identification

Mass spectral libraries (>700K spectra, >300K compounds):
automated identification of all peaks

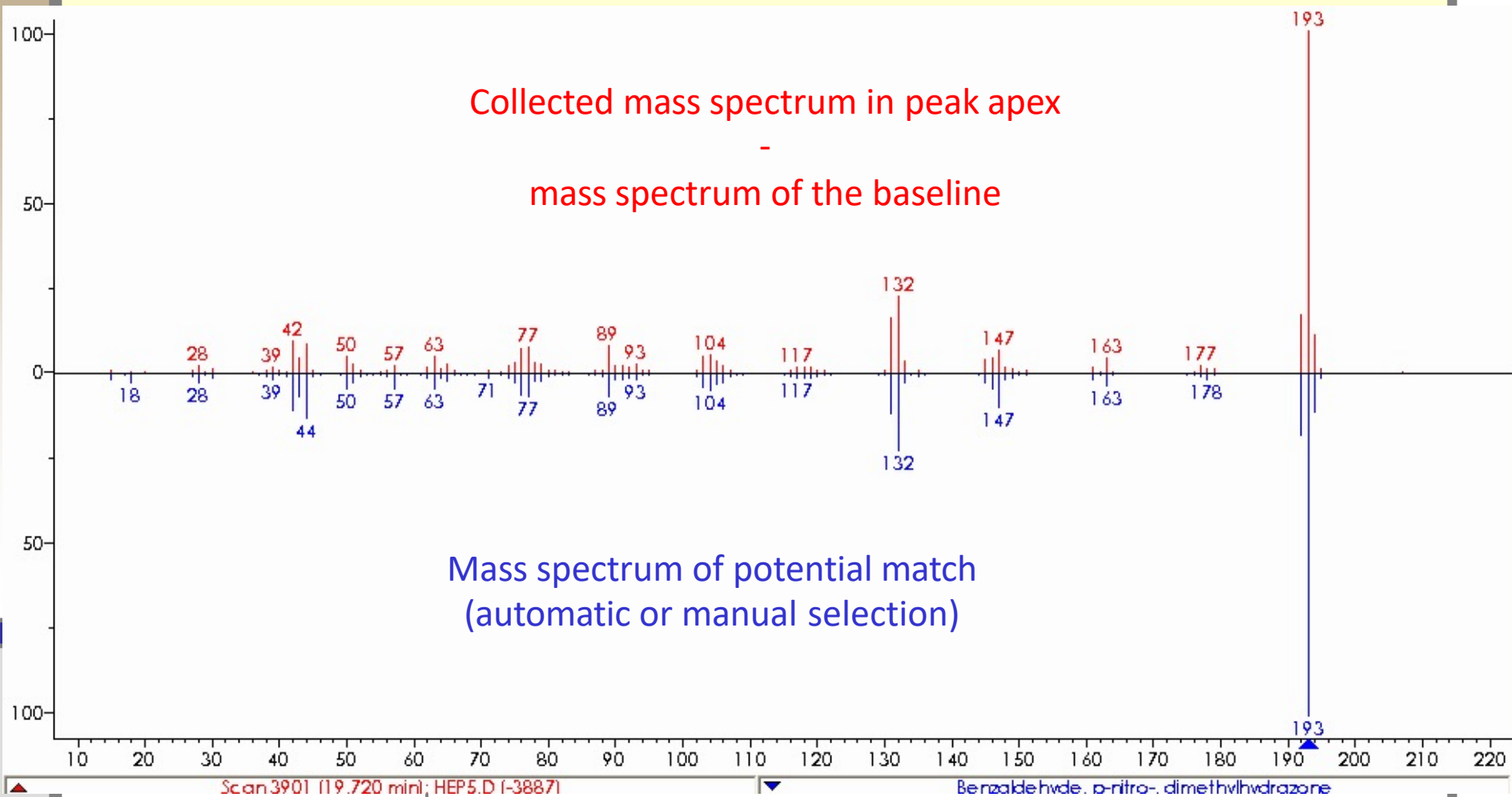
Deconvolution of peaks > detection and identification of several sub-peaks in larger or overlapping peaks using differences in mass spectra of each peak.

Every point of TIC has mass spectrum

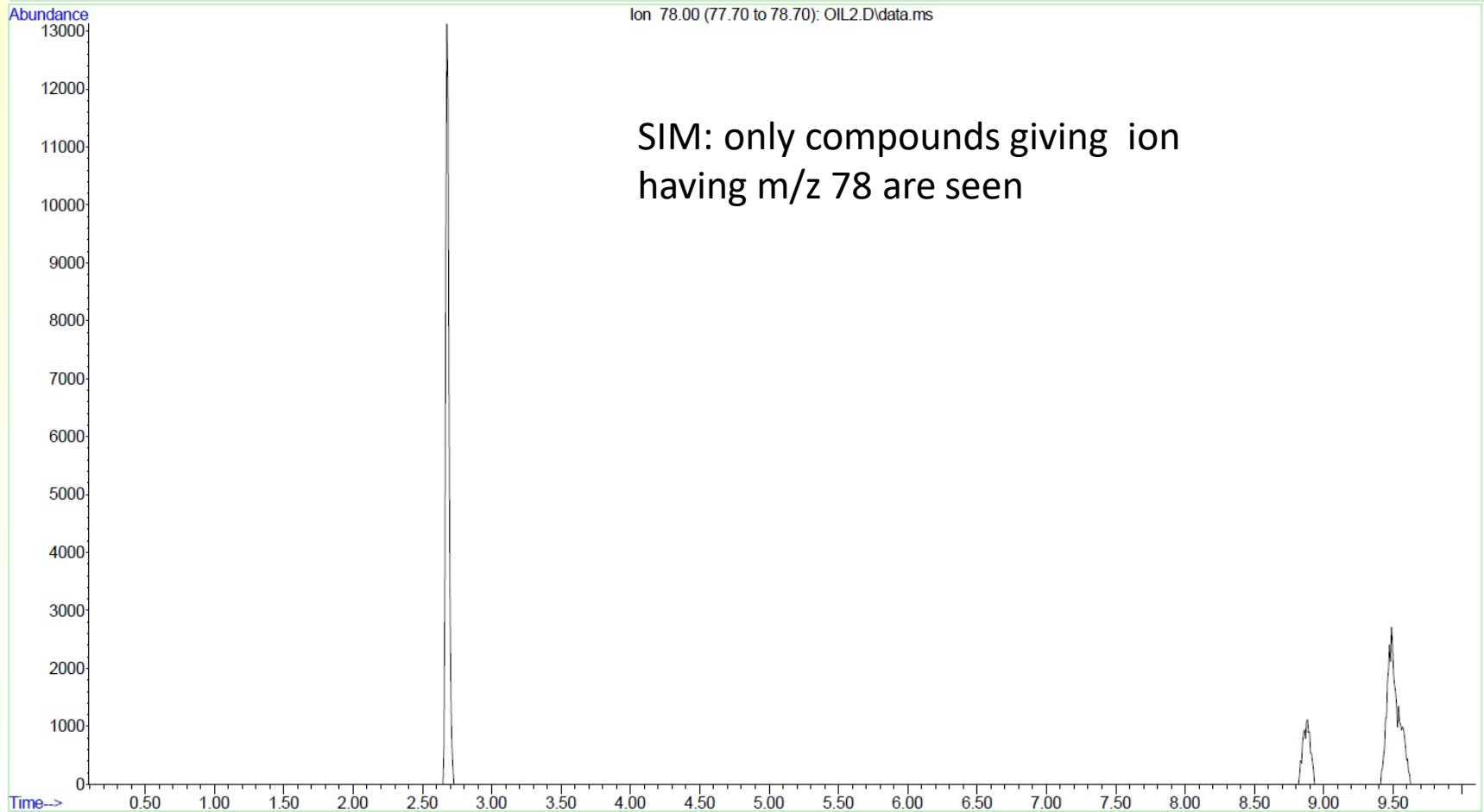


Every peak can be identified by MS only or by MS + RT (retention time)

Any peak can be identified using MS libraries



Difference of TIC and SIM chromatograms



MS detection modes

Scan in the desired m/z range:

efficient identification; quantification
by normalization; high baseline
noise;
low sensitivity (>10 pg);

VS

Selected ion monitoring (SIM):

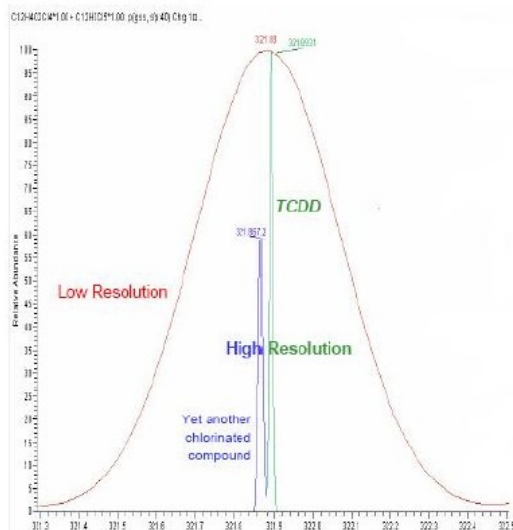
high selectivity;
low baseline noise;
high sensitivity (<1 pg);
identification by RT; confirmation
by MS ions ratios

OR

Synchronous SIM/Scan

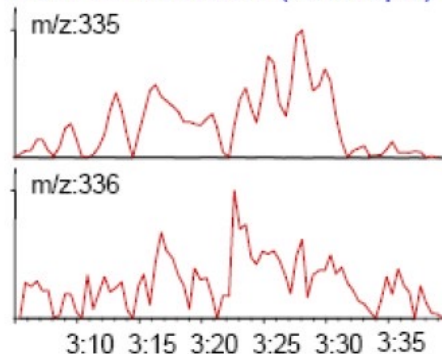
All above listed advantages;
Lower scanning rate and precision.

GC - High Resolution MS



**Increased selectivity of
high-resolution MS vs
low-resolution MS**

Low Resolution (Quadrupol)



High Resolution

