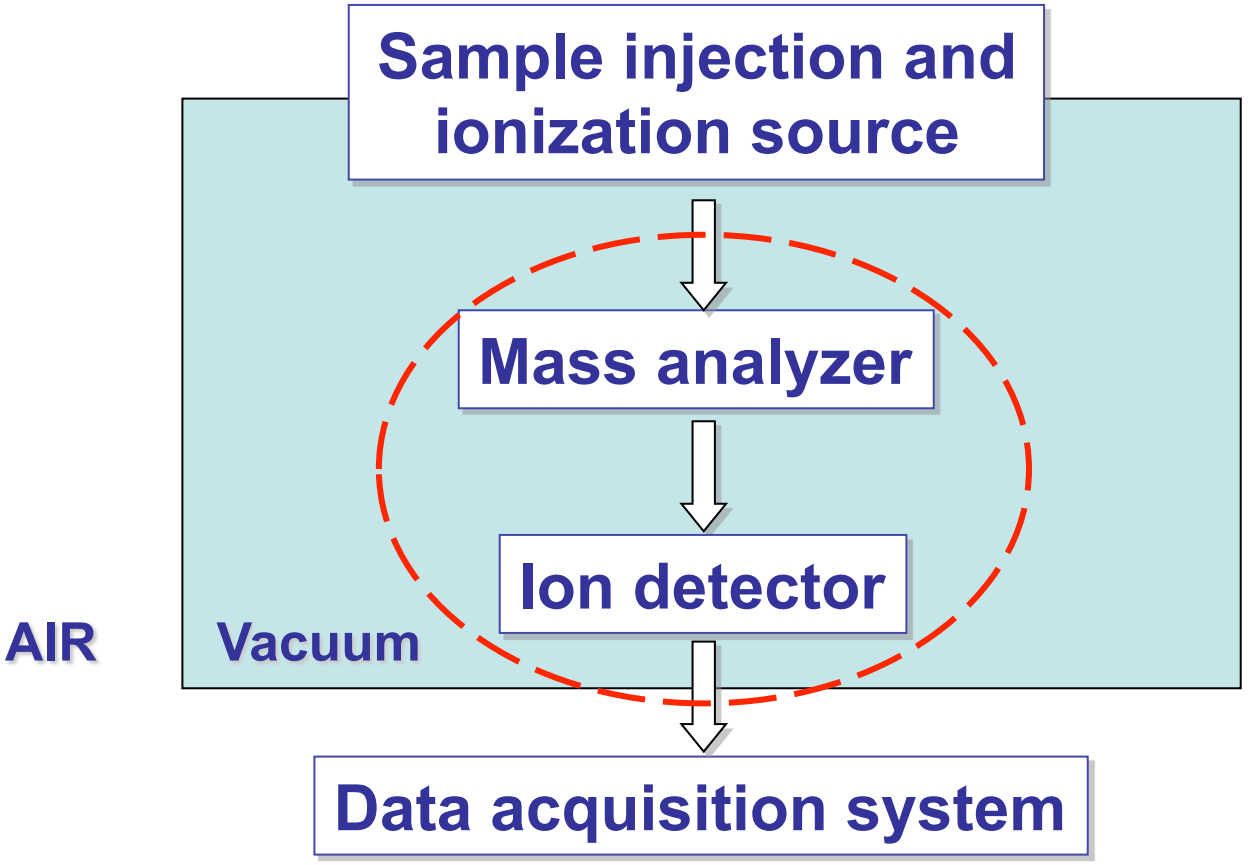
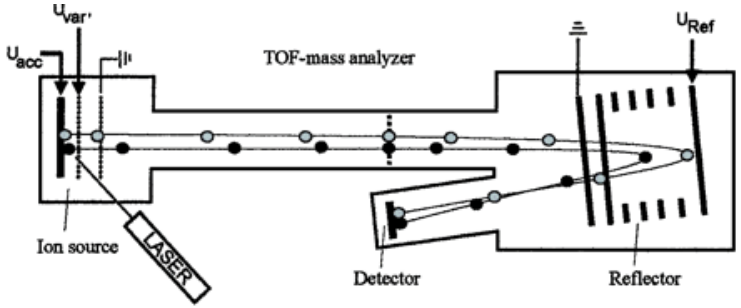
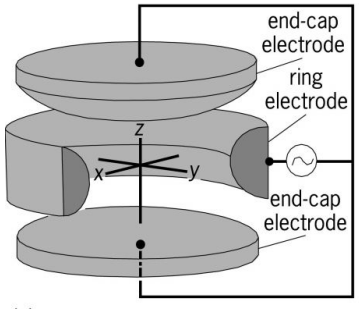
General Configuration of Mass Spectrometer

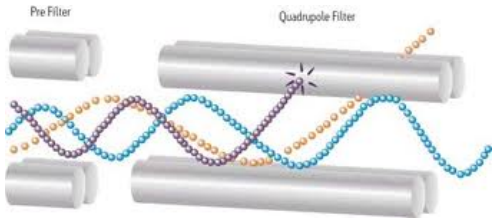


Important Mass Analyzers

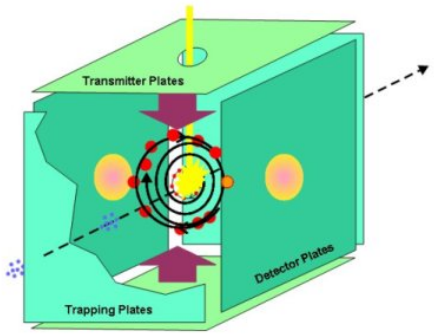


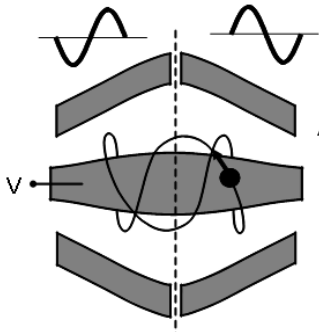
Time-of-Flight (TOF)



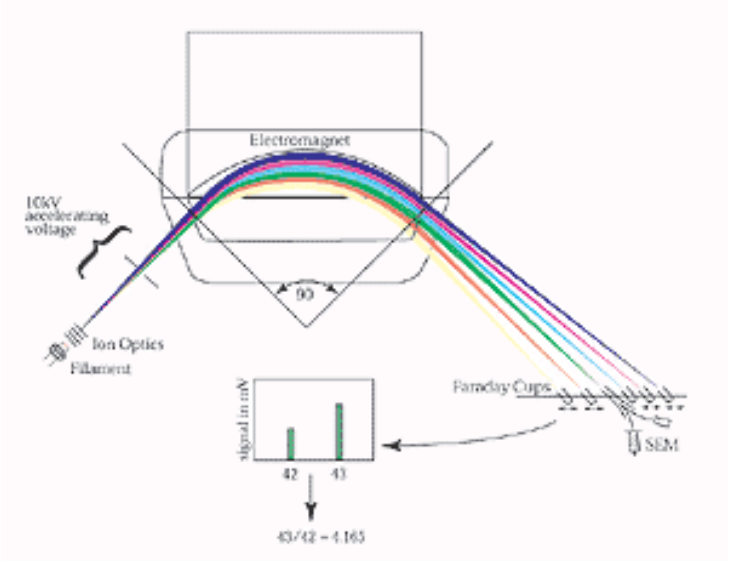


Ion Trap/Quadrupole



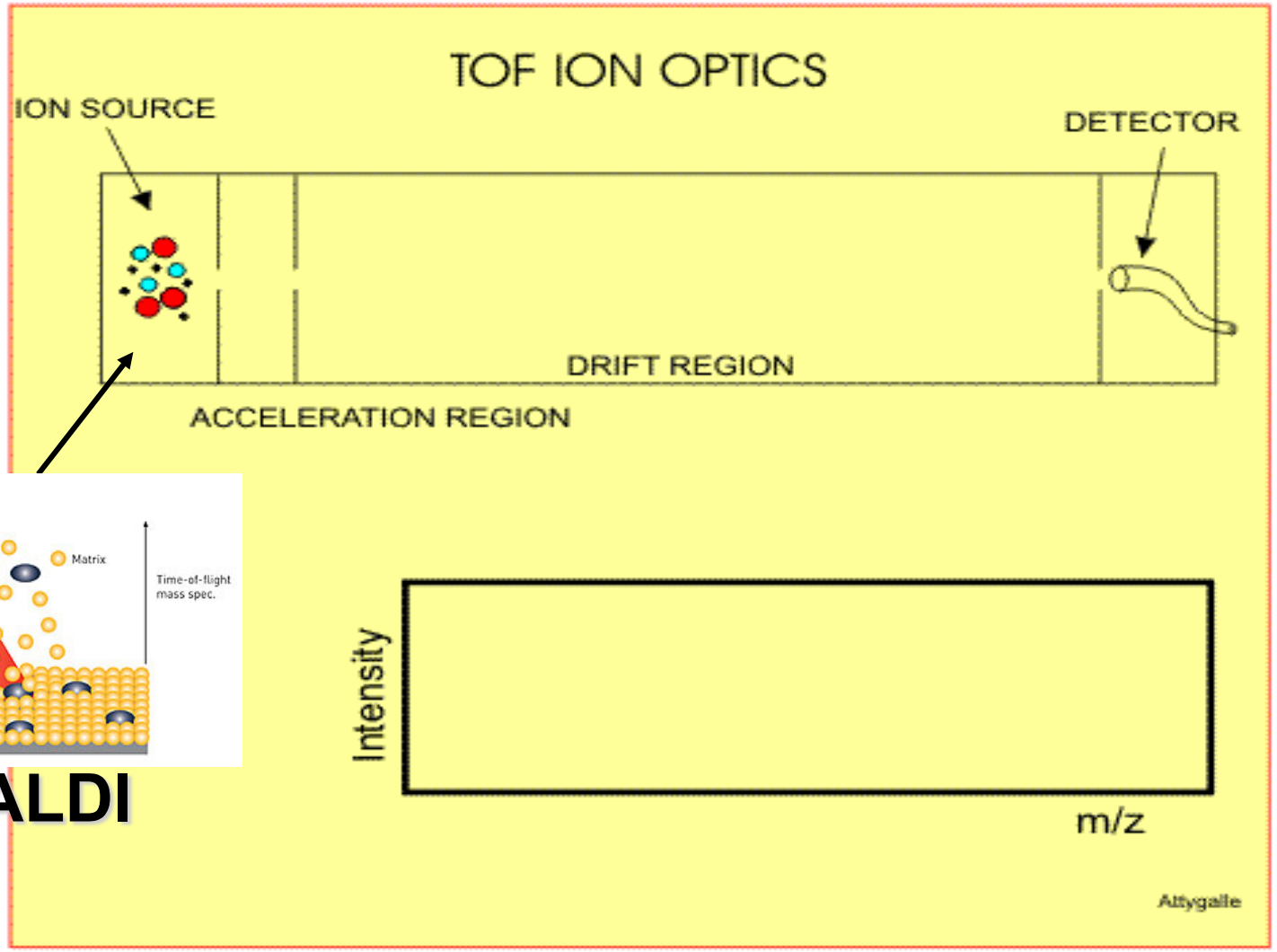


Fourier-Transform Mass Analyzer



Magnet Sector

Time-Of-Flight Mass Analyzer (TOF)



MALDI

MALDI-TOFMS

Principle

Energy conservation between potential and kinetic energies

Kinetic energy (*K.E.*) = *qV*

$K.E. = (1/2)\, m\, v^2 = qV$

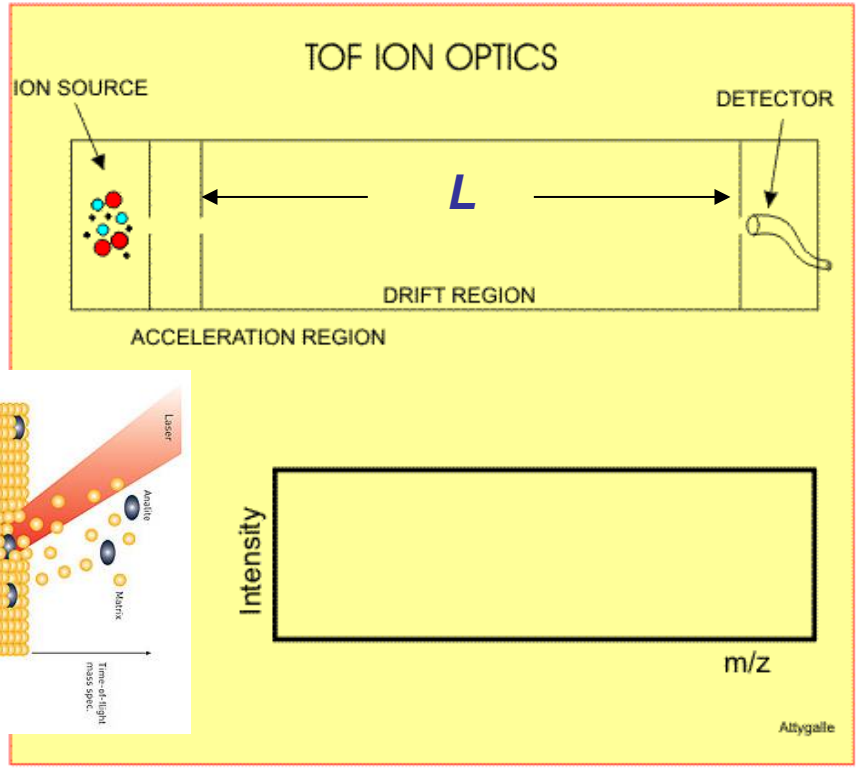
$v = (2qV/m)(1/2)$

The traveling time (*t*) through the drift region is *L/v* where *L* is the length of the drift region.

$t = L / (2V/m/q)^{1/2}$

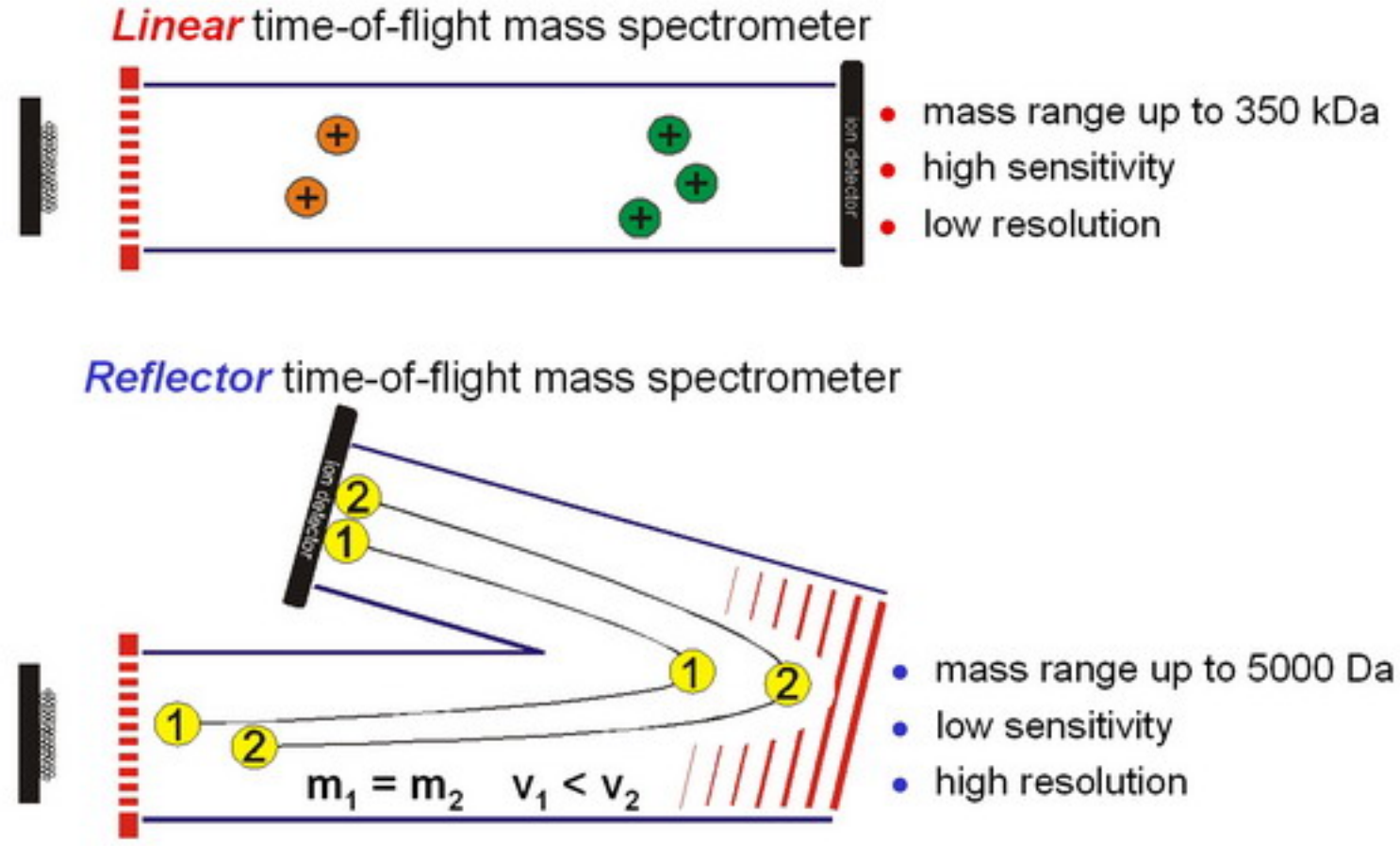
Parameters:

q = electric charge on ions
V = Acceleration voltage for ions
m = molecular weight of ions
v = velocity of ions
t = traveling time
L = drift length



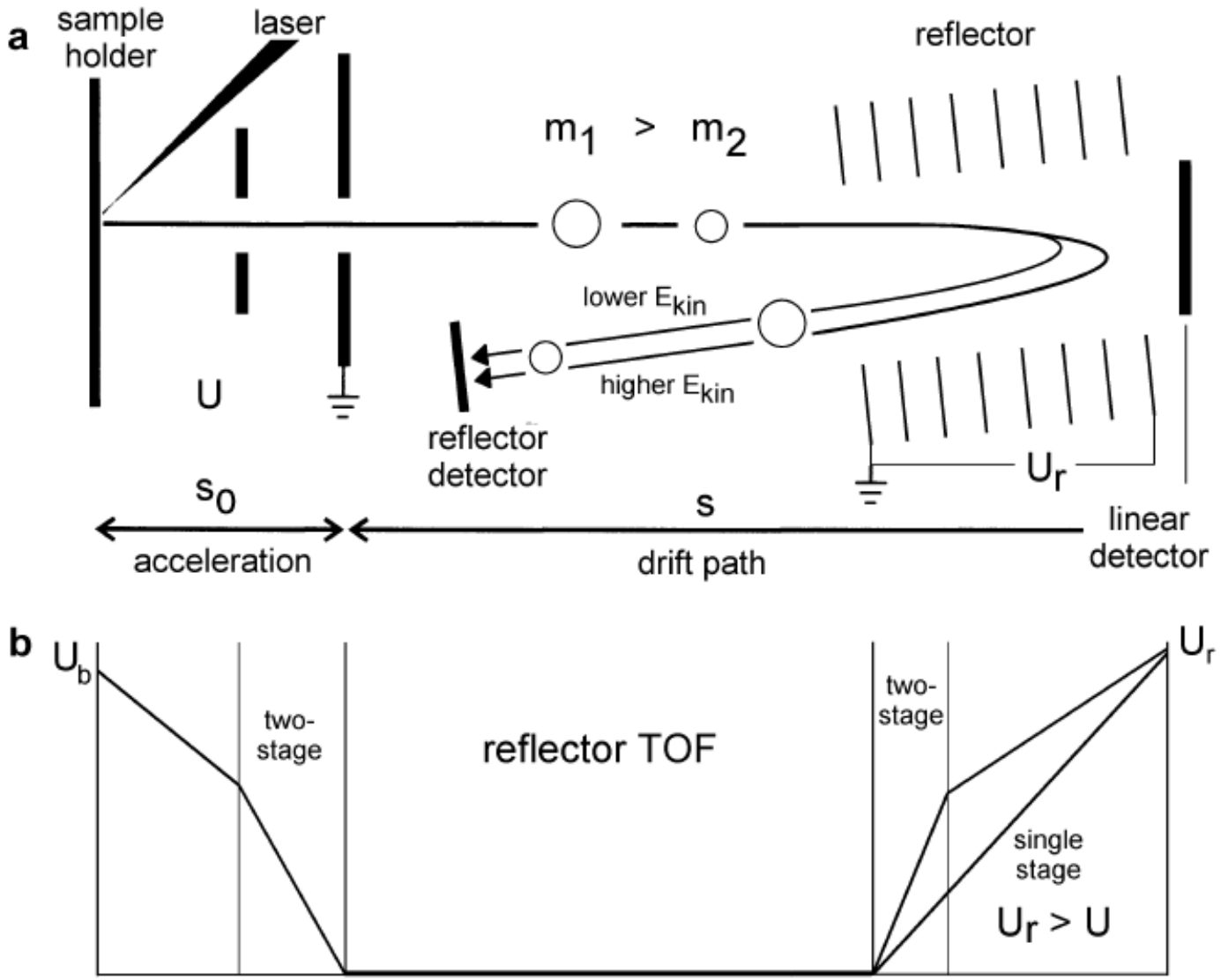
Commercial TOF

Linear and reflector TOF MS

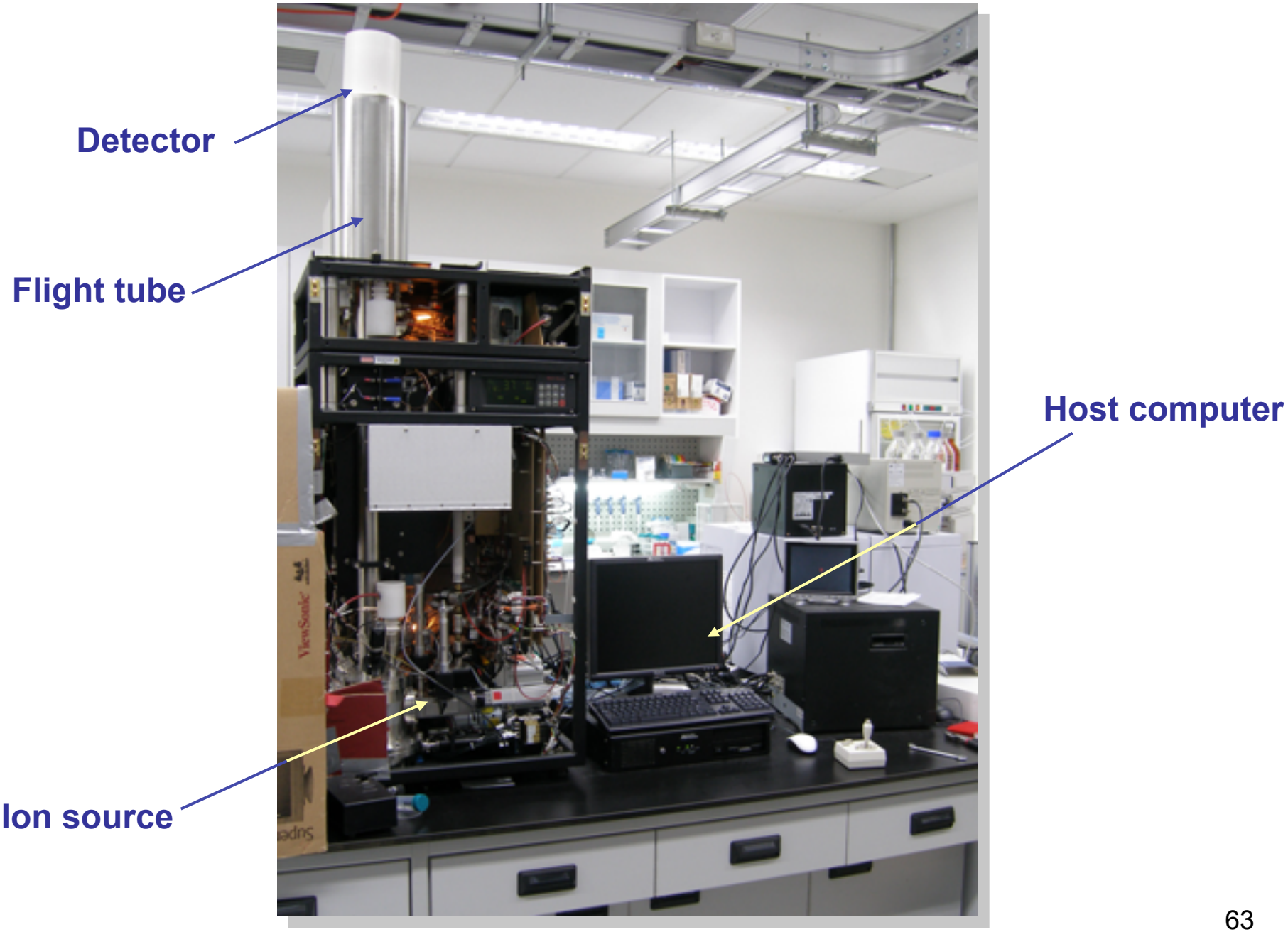


AnagnosTec

Commercial TOF

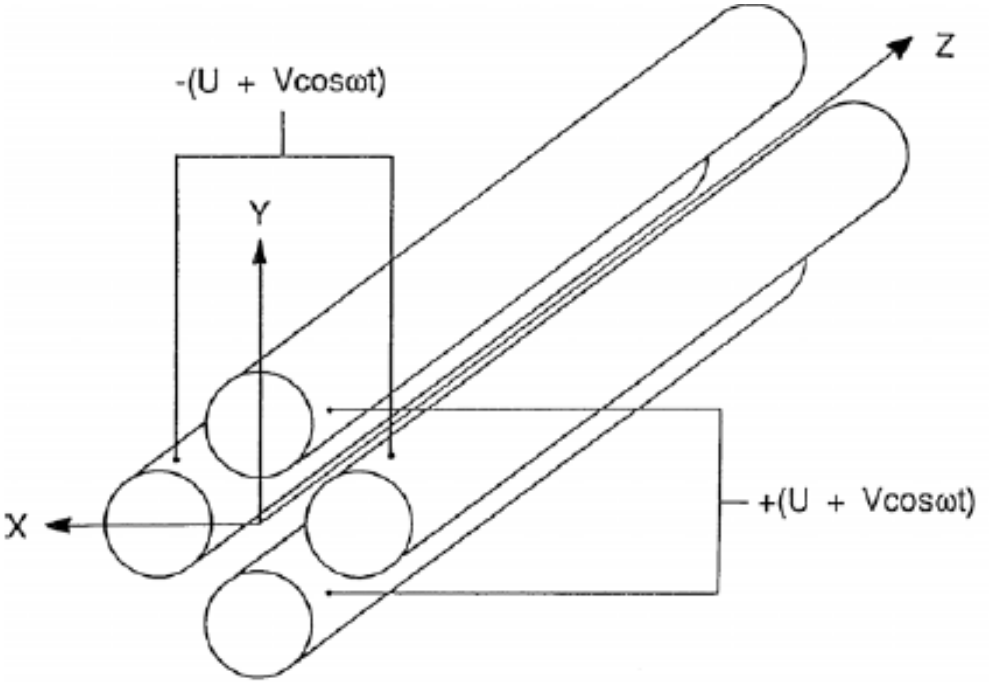


J. H. Gross, Mass Spectrometry A Textbook



MALDI-TOF MS (*Apply Biosystem Inc., USA*)

Quadrupole Mass Filter



Equation of ion motion (Mathieu eq.)

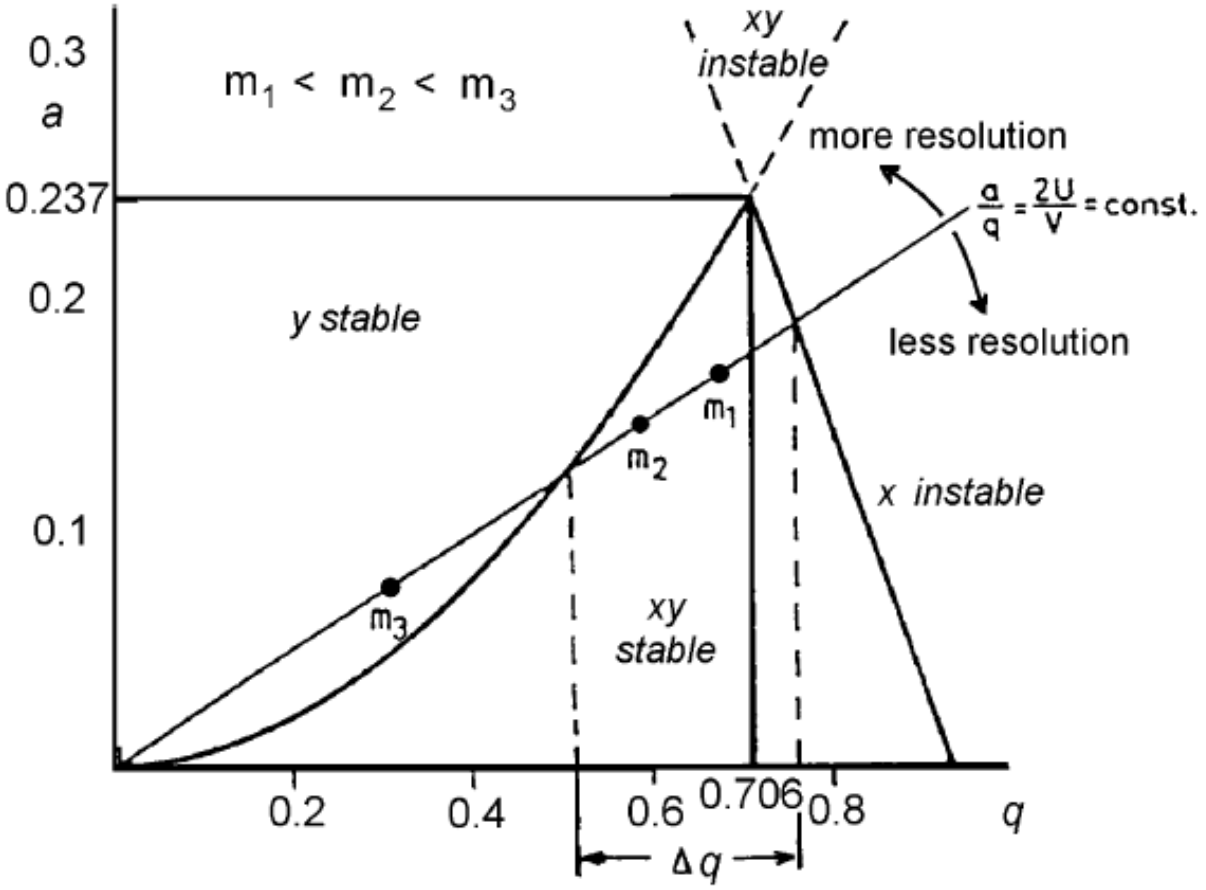
$$\frac{d^2x}{dt^2} + \frac{e}{m_i {r_0}^2}(U + V\cos\omega t)x = 0$$

$$\frac{d^2y}{dt^2} - \frac{e}{m_i {r_0}^2}(U + V\cos\omega t)y = 0$$

$$a_x = -a_y = \frac{4eU}{m_i {r_0}^2\omega^2}, \quad q_x = -q_y = \frac{2eV}{m_i {r_0}^2\omega^2}$$

J. H. Gross, Mass Spectrometry A Textbook

Quadrupole Mass Filter



$$a_x = -a_y = \frac{4eU}{m_i r_0^2 \omega^2}, \quad q_x = -q_y = \frac{2eV}{m_i r_0^2 \omega^2}$$

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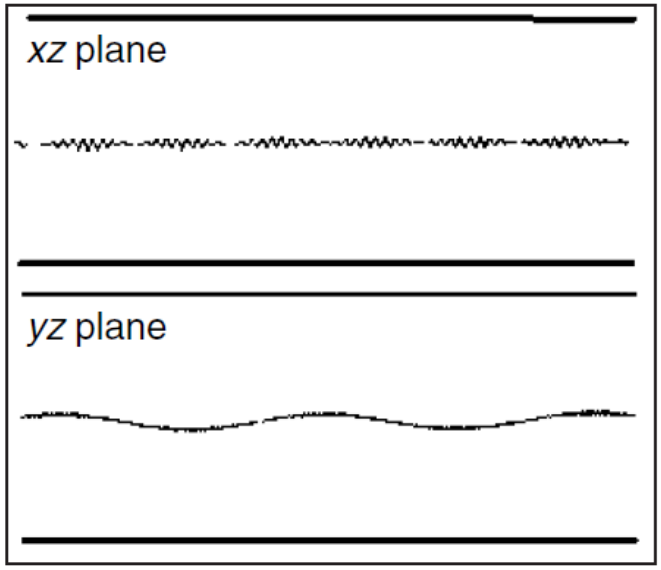
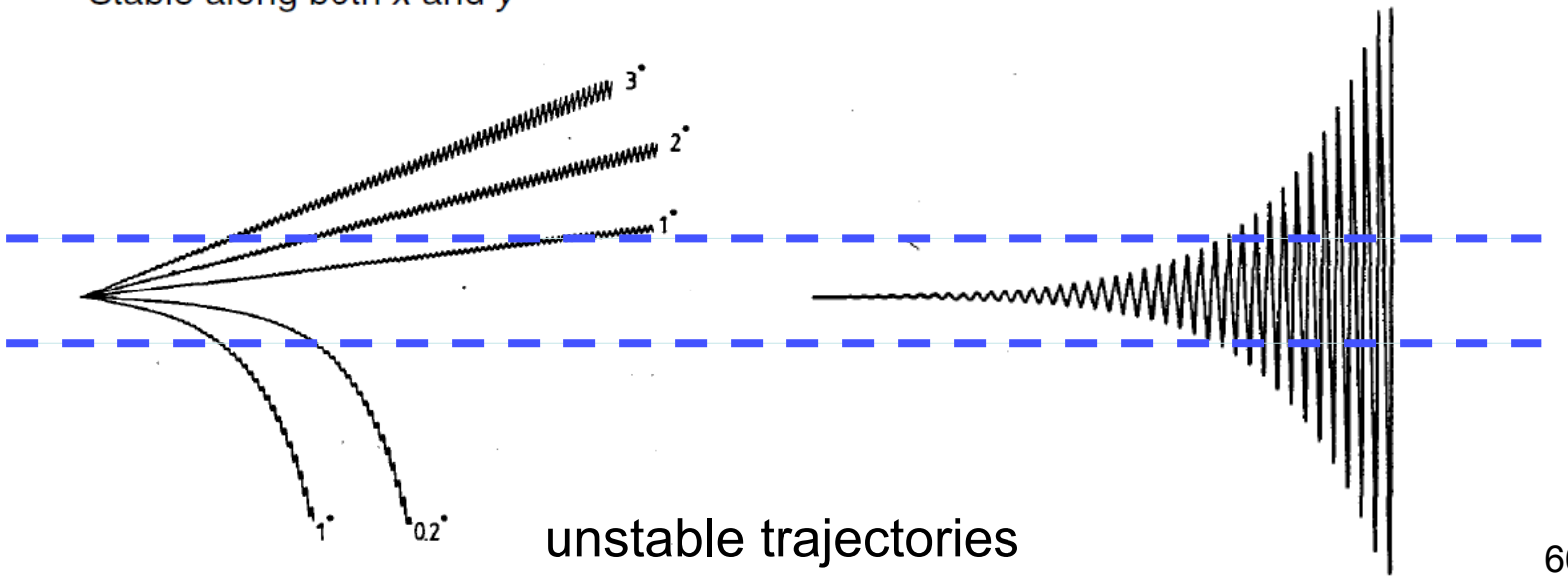
Quadrupole Mass Filter



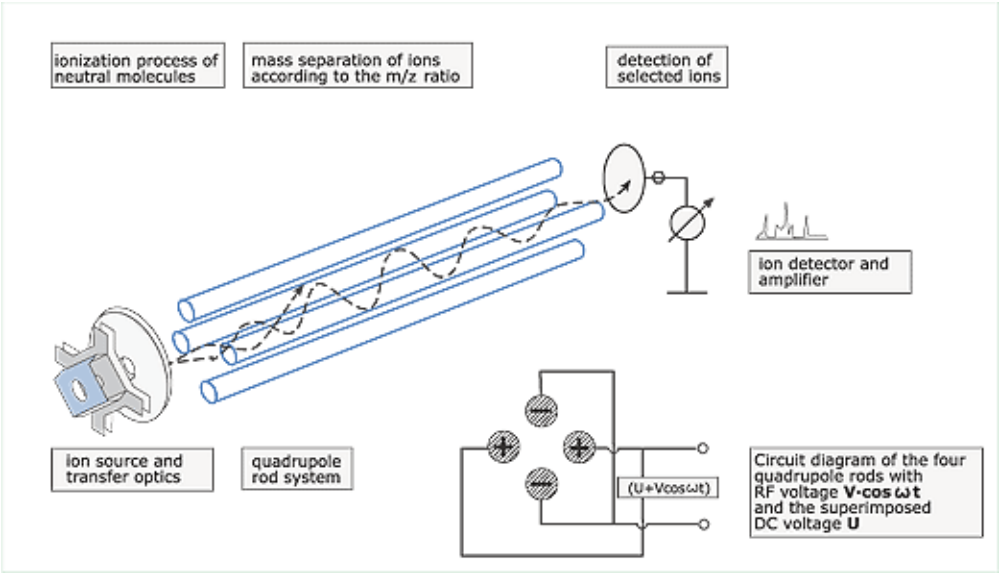
Stable along both *x* and *y*

stable trajectory

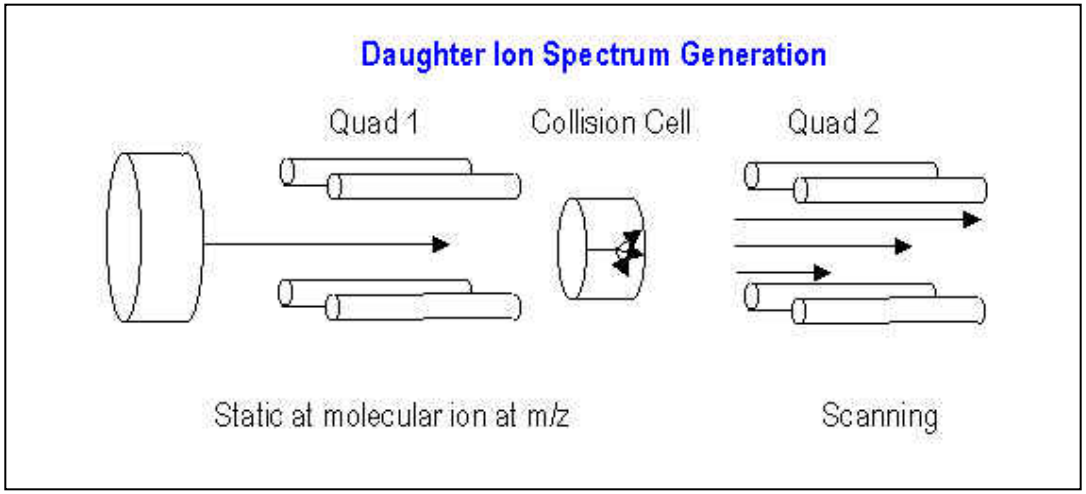


unstable trajectories

Quadrupole Rods and Triple-Quad MS

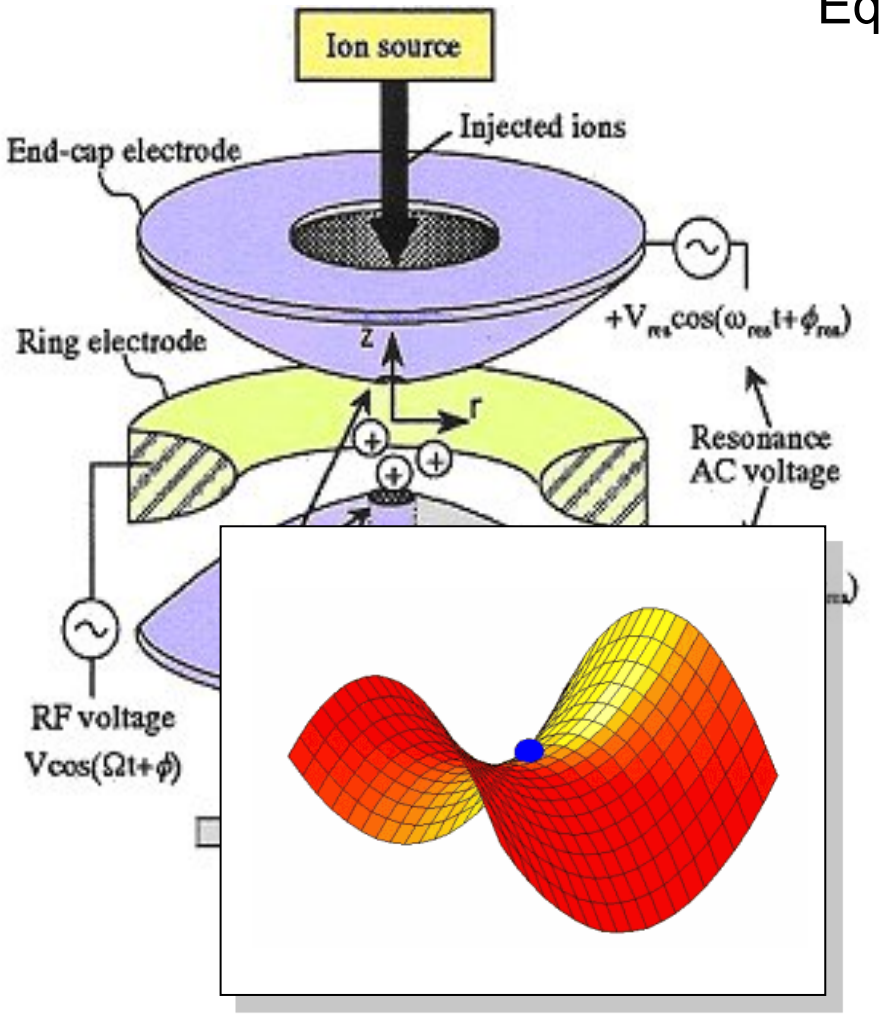


Inprocess Instruments



Dr. Graeme T. Clark , University Child Health,Southampton General Hospital,

Quadrupole Ion Trap



$q_z \leq 0.908$

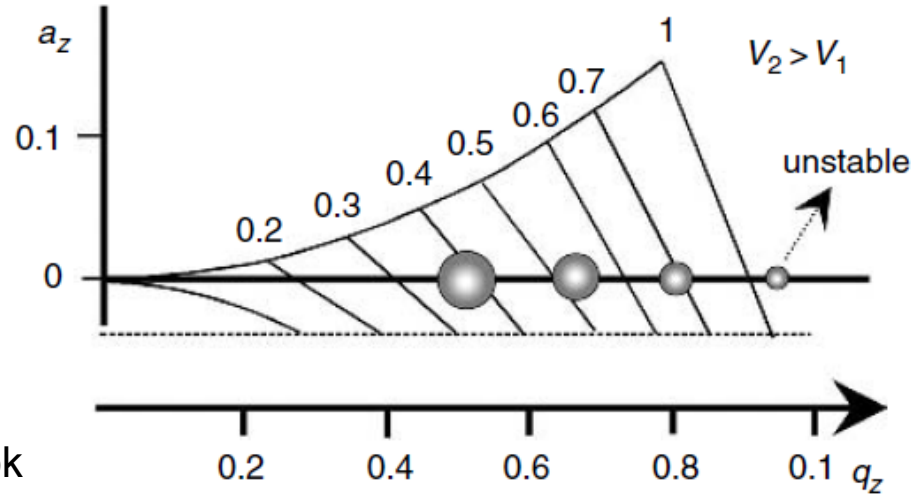
Equation of ion motion (Mathieu eq.)

$$\frac{d^2z}{dt^2} - \frac{4e}{m_i\left(r_0^2 + 2z_0^2\right)}(U - V\cos\Omega t)z = 0$$

$$\frac{d^2r}{dt^2} + \frac{2e}{m_i\left(r_0^2 + 2z_0^2\right)}(U - V\cos\Omega t)r = 0$$

$$a_z = -2a_r = -\frac{16eU}{m_i\left(r_0^2 + 2z_0^2\right)\Omega^2}$$

$$q_z = -2q_r = \frac{8eV}{m_i\left(r_0^2 + 2z_0^2\right)\Omega^2}$$



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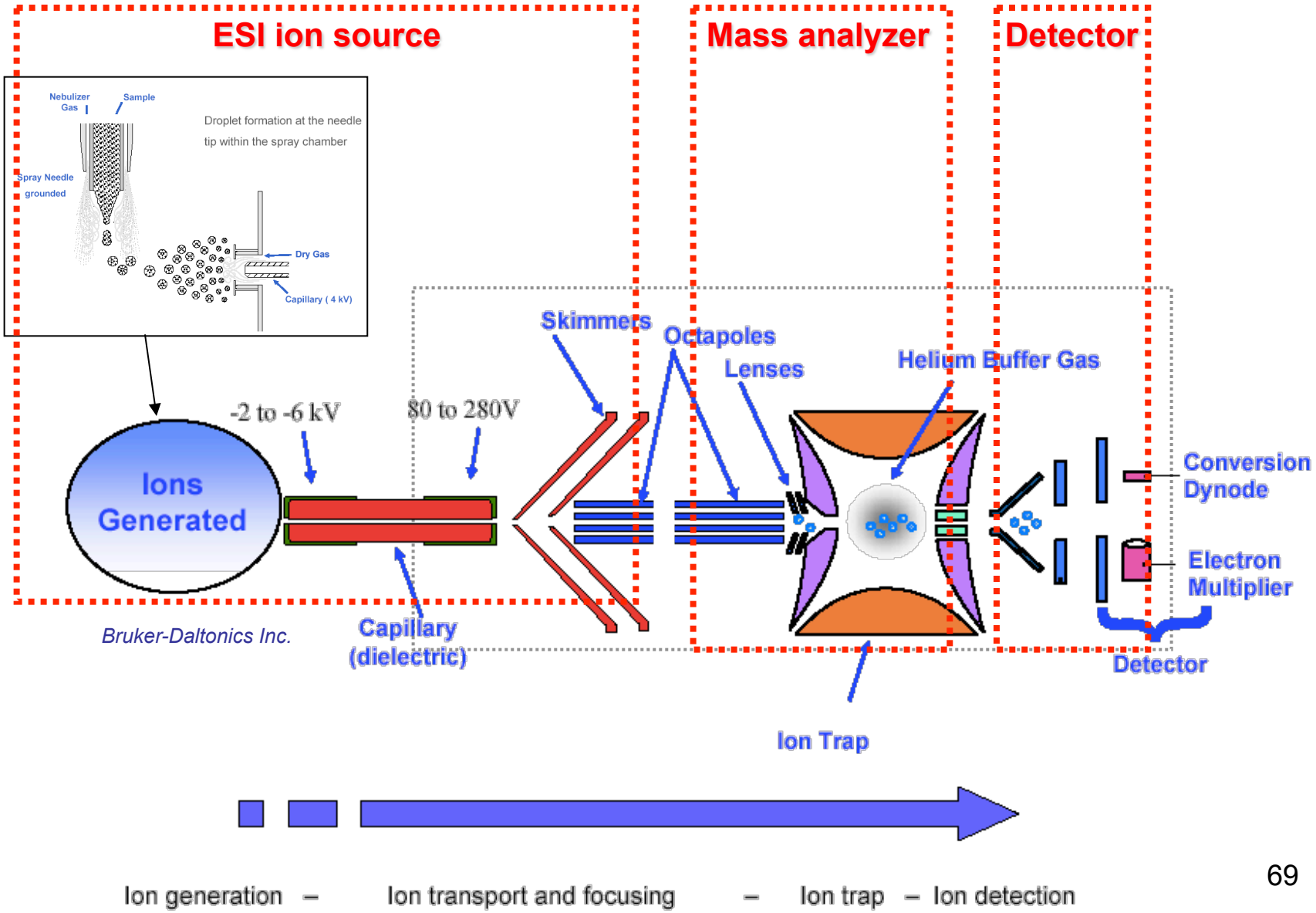
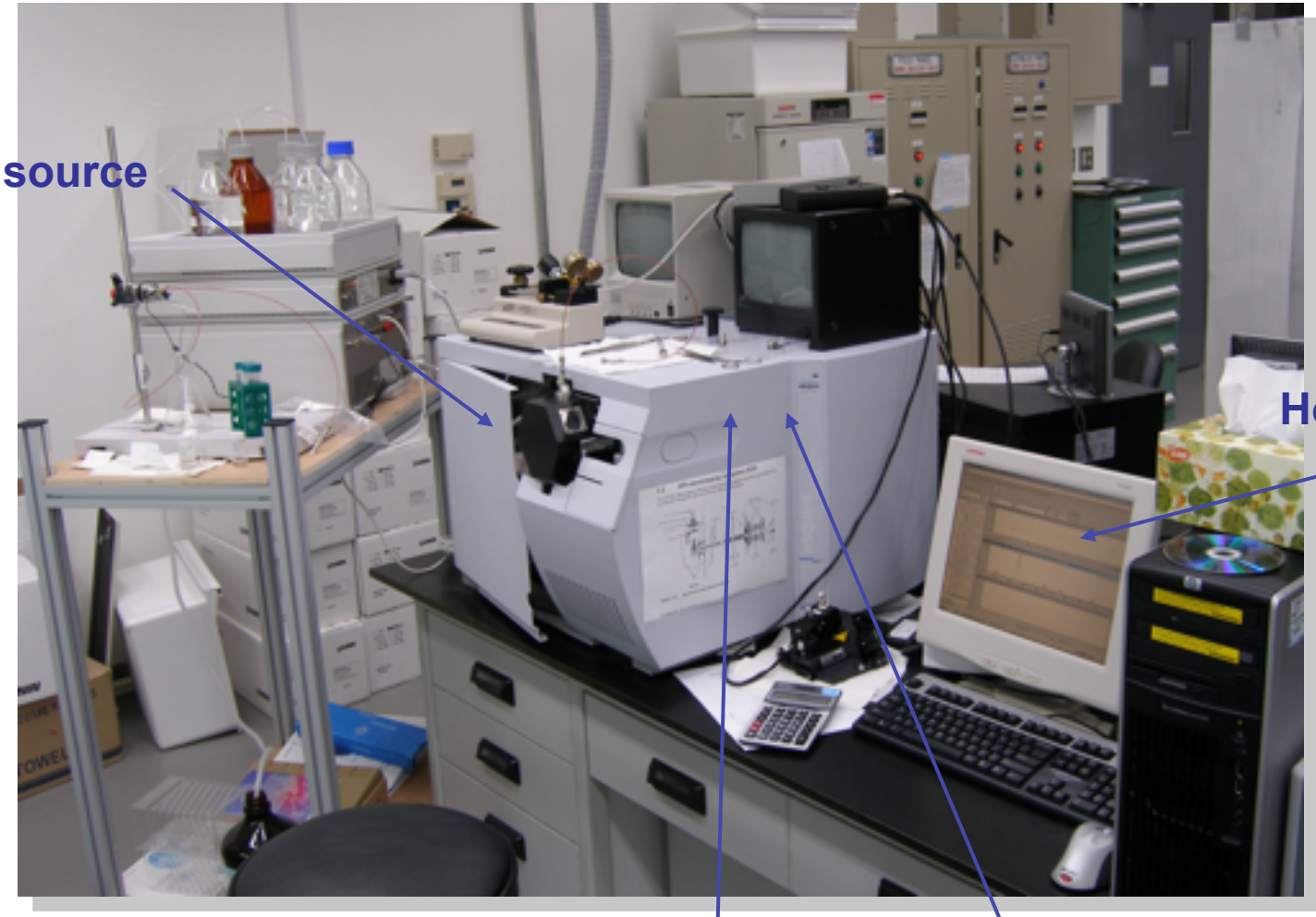
Ion Trap (with ESI source)

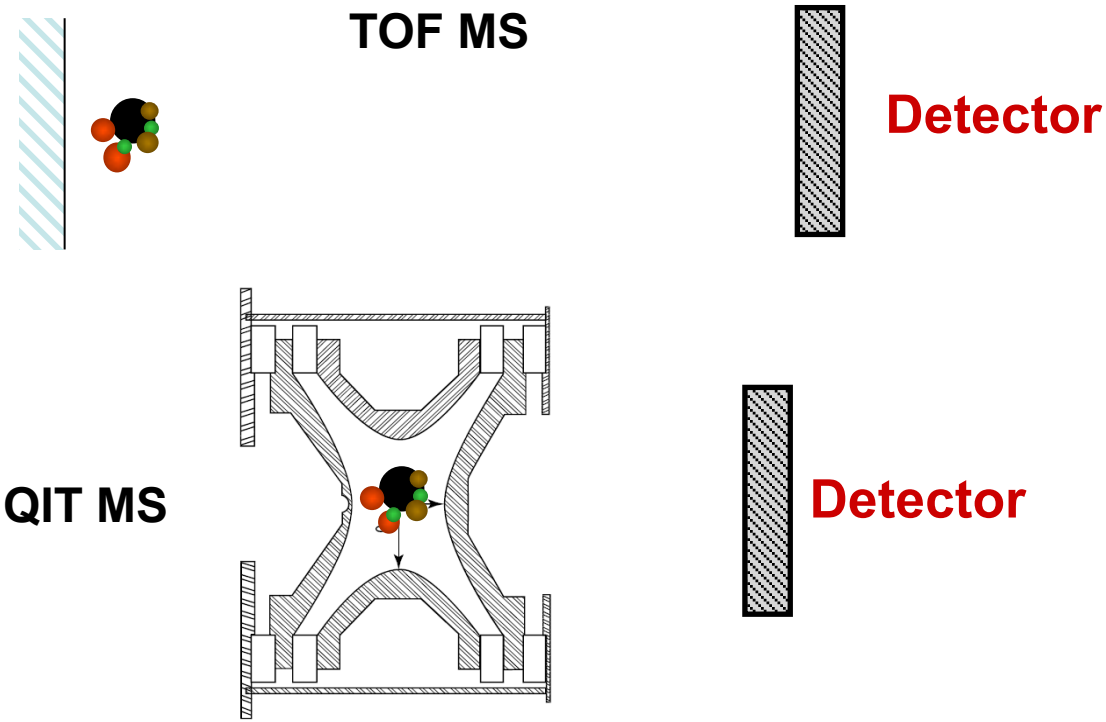


ESI-Q MS (*Bruker-Daltonics Inc., USA*)

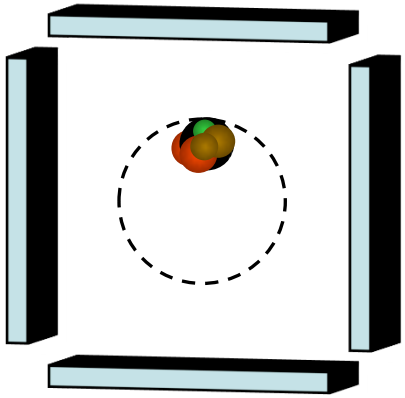


Sequential V.S. Simultaneous Detection

Sequential Detection

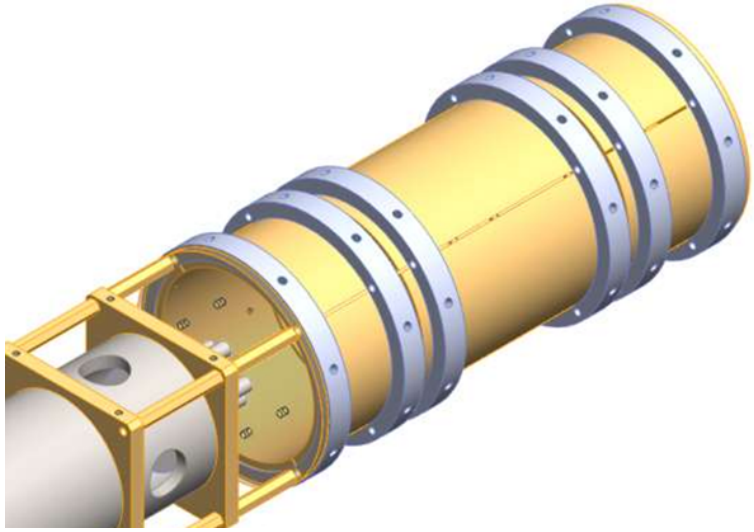


Simultaneous Detection
(Fourier-Transform MS)

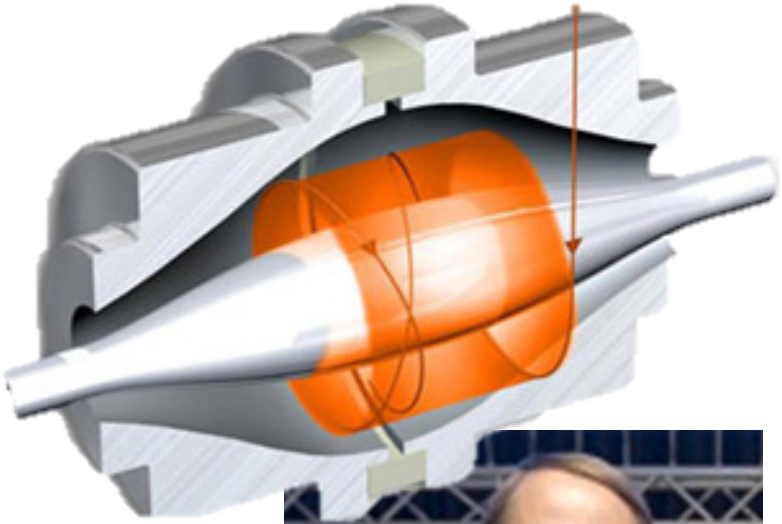


Commercial FT Mass Spectrometers

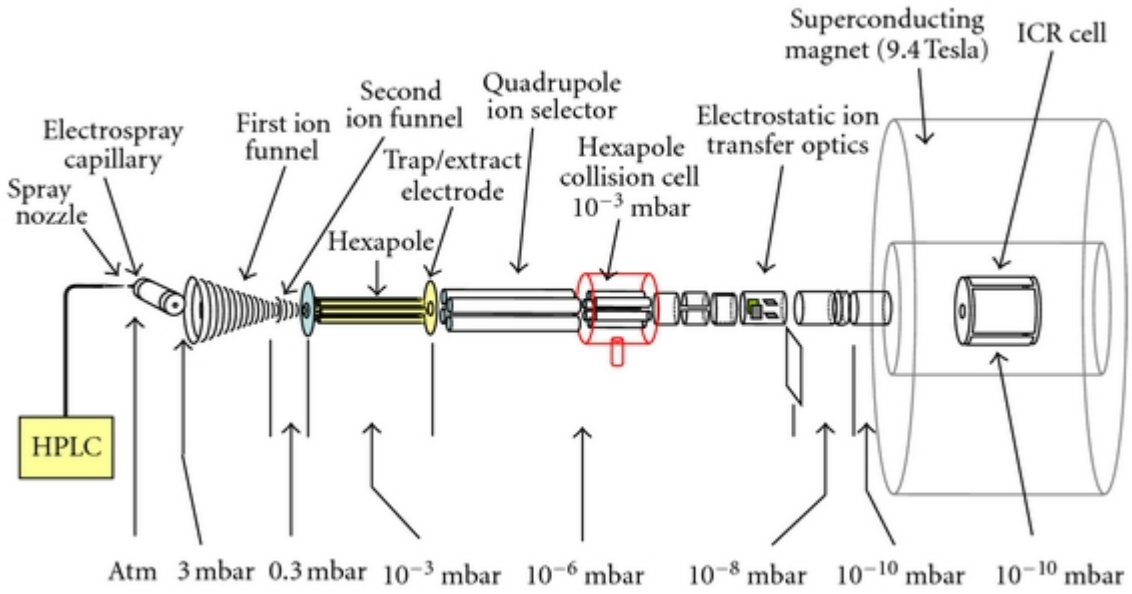
FT-ICR



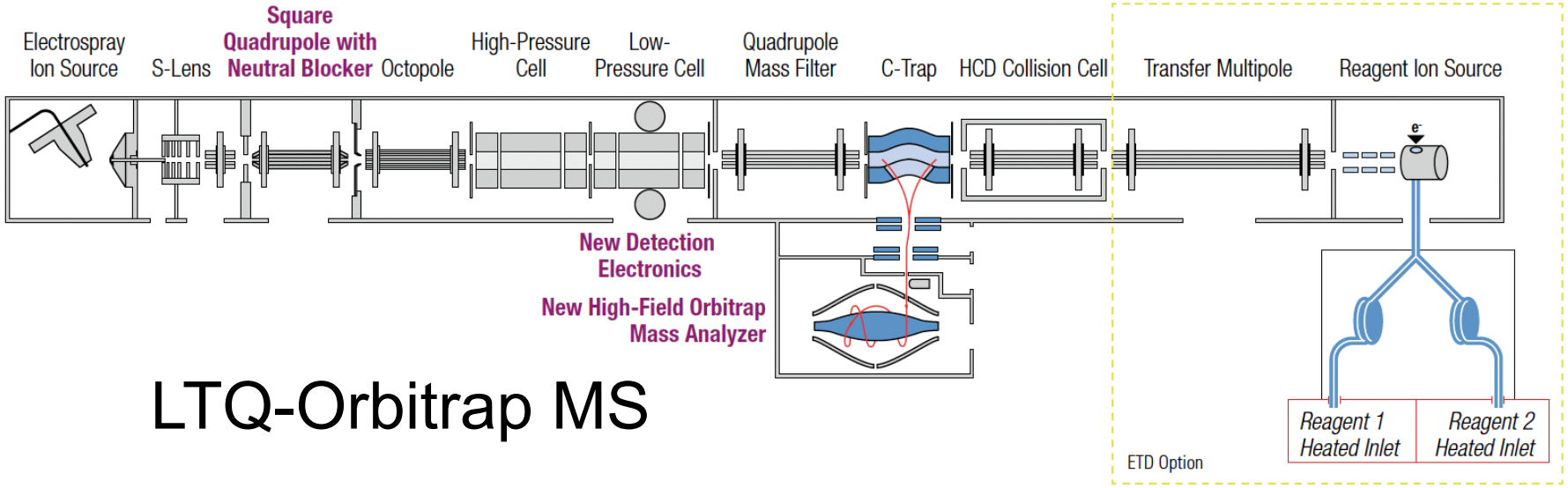
Orbitrap



Configuration of FTMS



FT-ICR MS

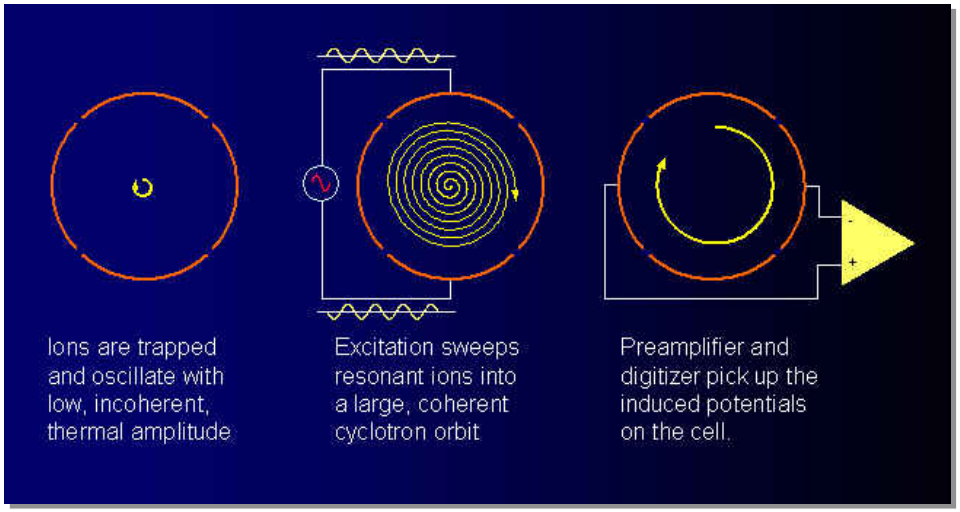


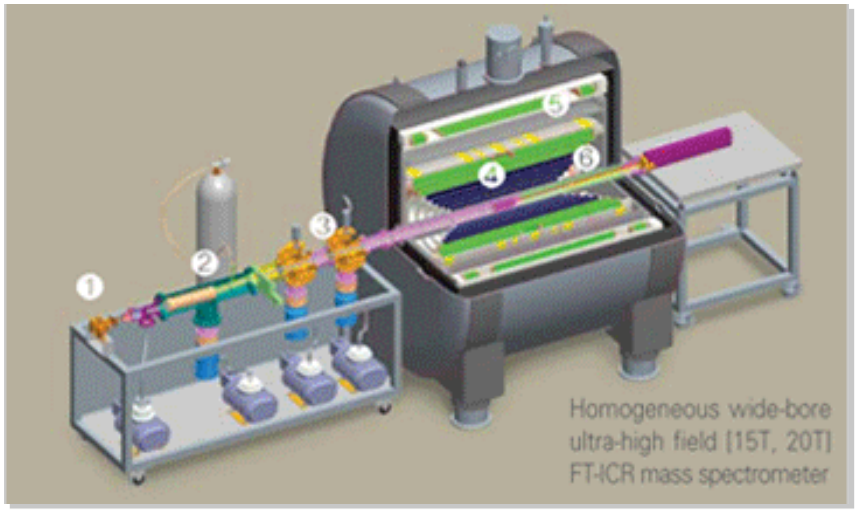
LTQ-Orbitrap MS

FT-ICRMS

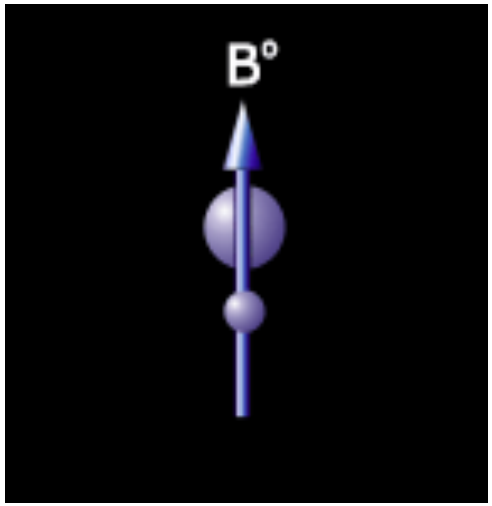
Fourier-Transform — A method for data handling, which converts time-domain signal to frequency-domain data using Fourier transformation method.

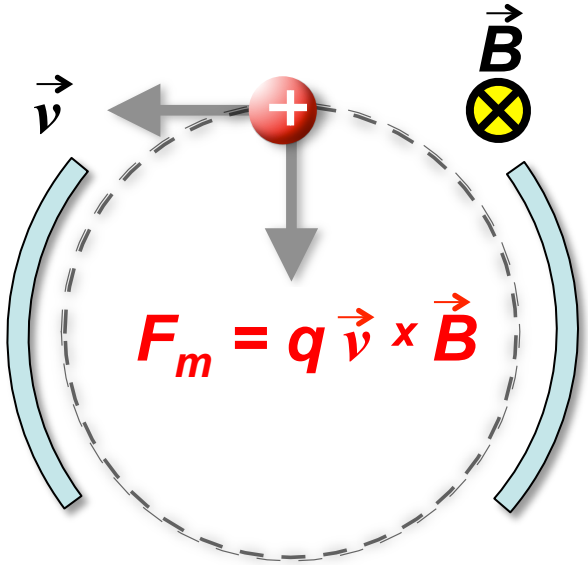
Ion-Cyclotron-Resonance — High resolution ion recognition by detecting the frequency of ion cyclotron motion in high magnetic field.





Ion-Cyclotron Motion in High Magnetic Field





$$F_m = m\vec{v}^2/r = q\,\vec{v}\vec{B}$$

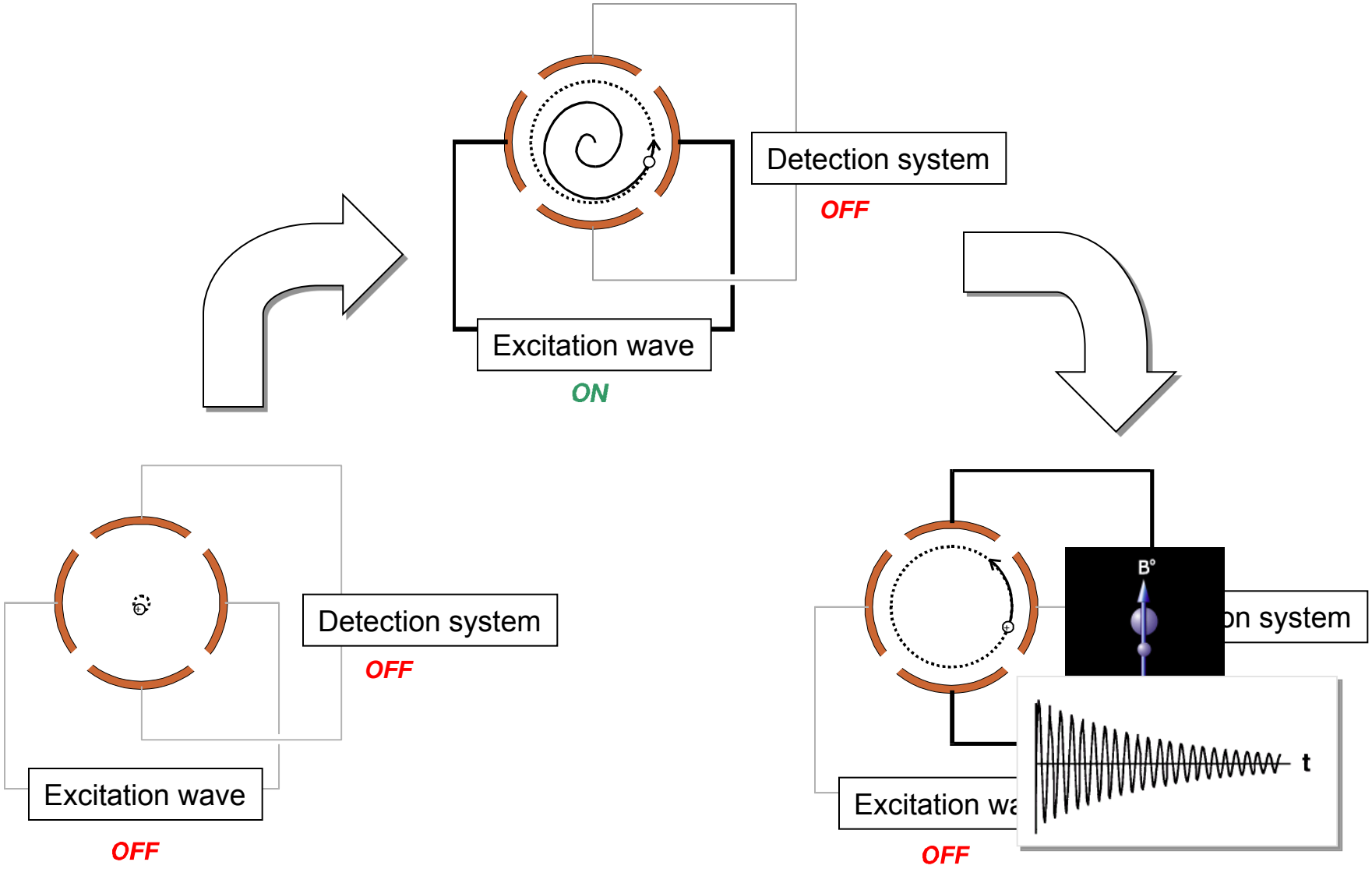
$$m\,\vec{v}/r = m\omega_c = q\vec{B}$$

$$\omega_c = (q/m)\,\vec{B}$$

$$\nu_c = \omega_c / 2\pi$$

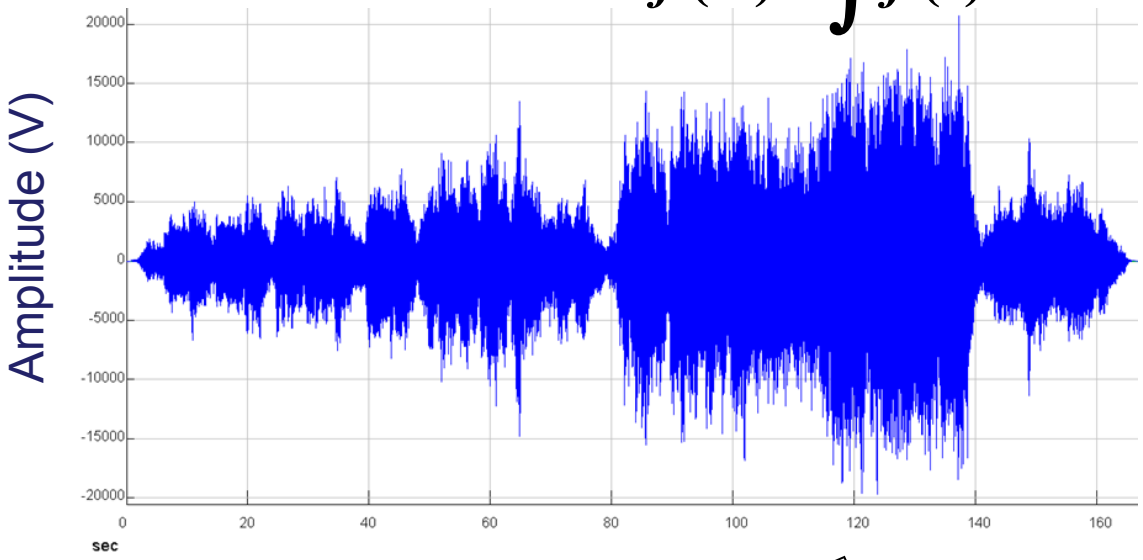
An ion moving in the presence of a spatially uniform magnetic field B is subject to a force (F).

Ion Cyclotron Motion:
Excitation and Detection



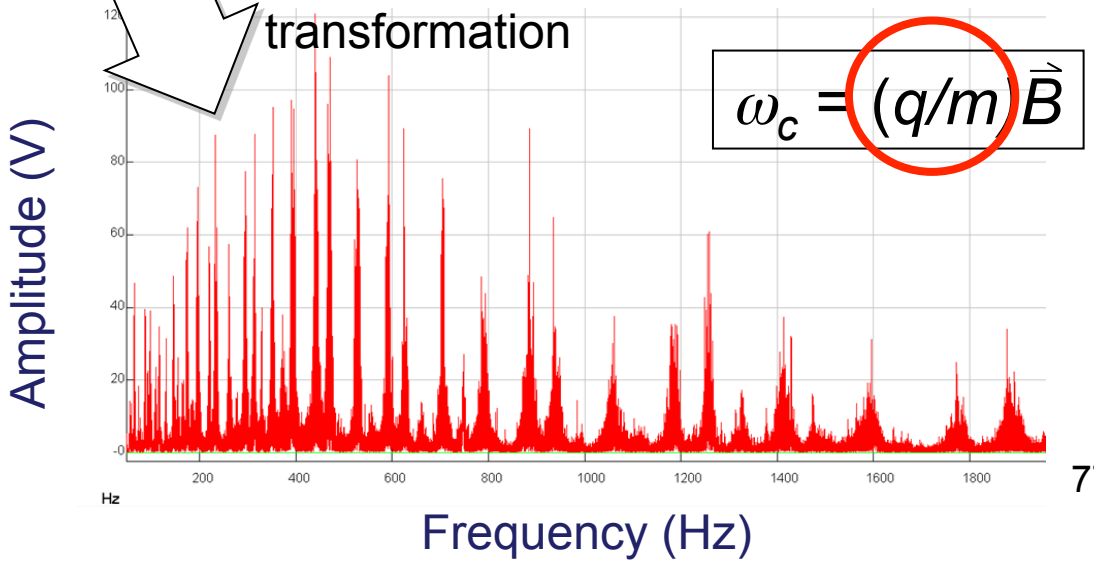
The Concept of Fourier-Transform in MS

$$f(\omega) = \int f(t) e^{-i\omega t} dt$$



signal in time-domain (時域)

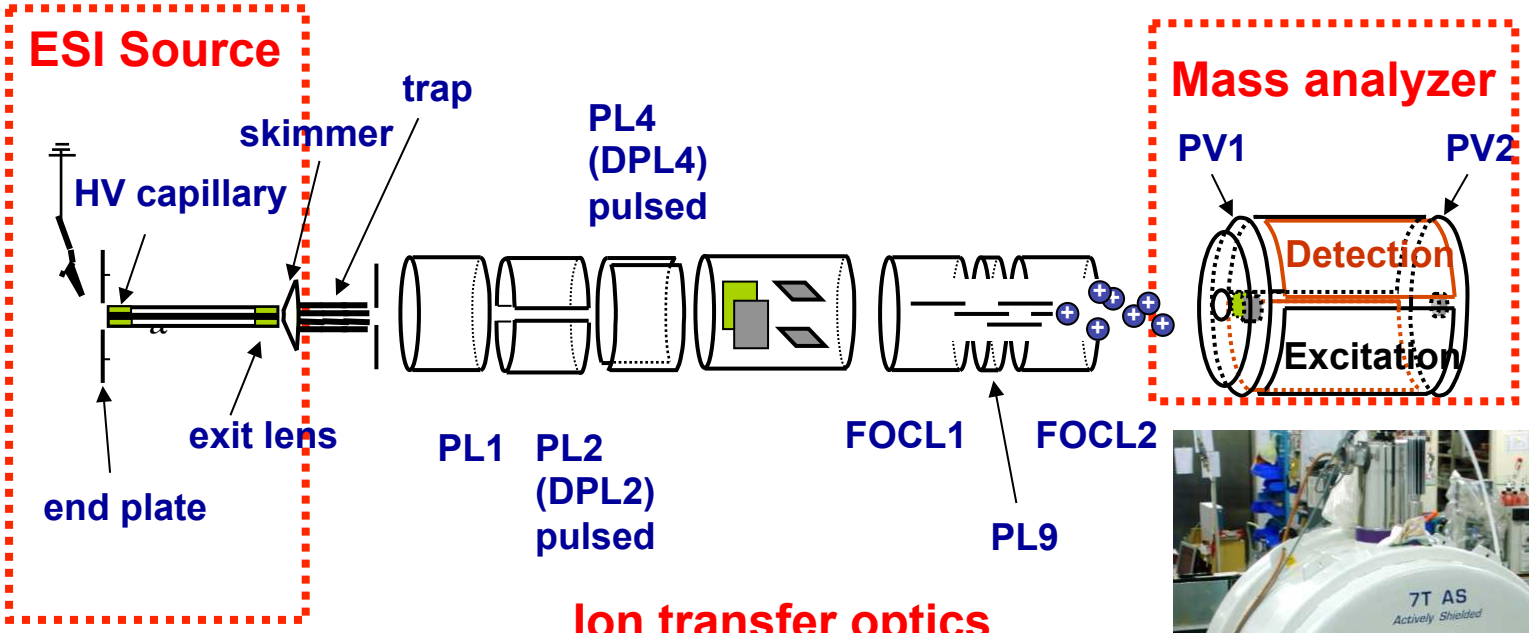
Fourier transformation

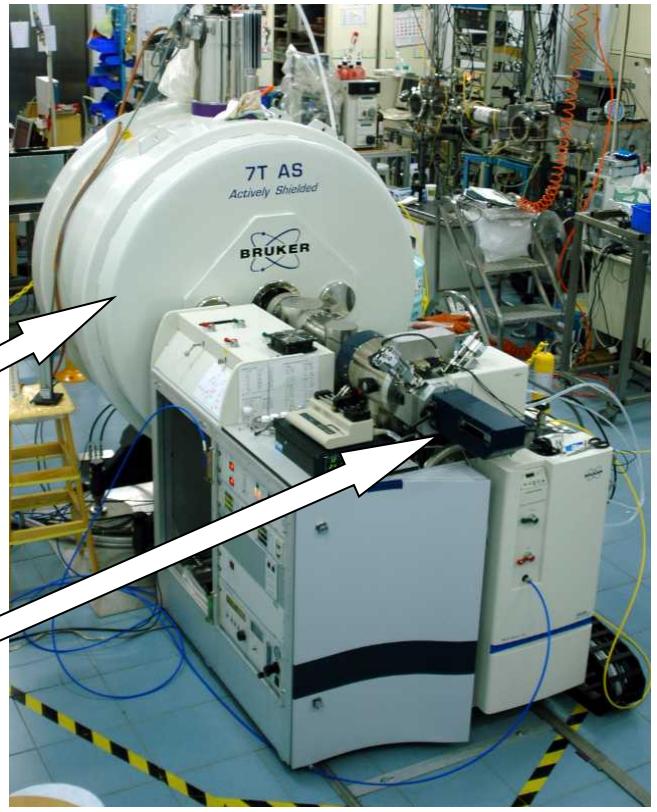


$$\omega_c = (q/m)\vec{B}$$

signal in frequency-domain (頻域)

Configuration of Commercial FT-ICRMS

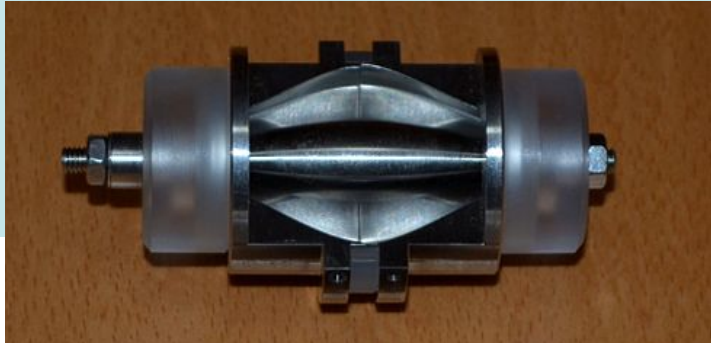




superconducting magnet

ion source

ORBITRAP



A. Makarov
Anal. Chem. 72 (6), 1156 (2000).

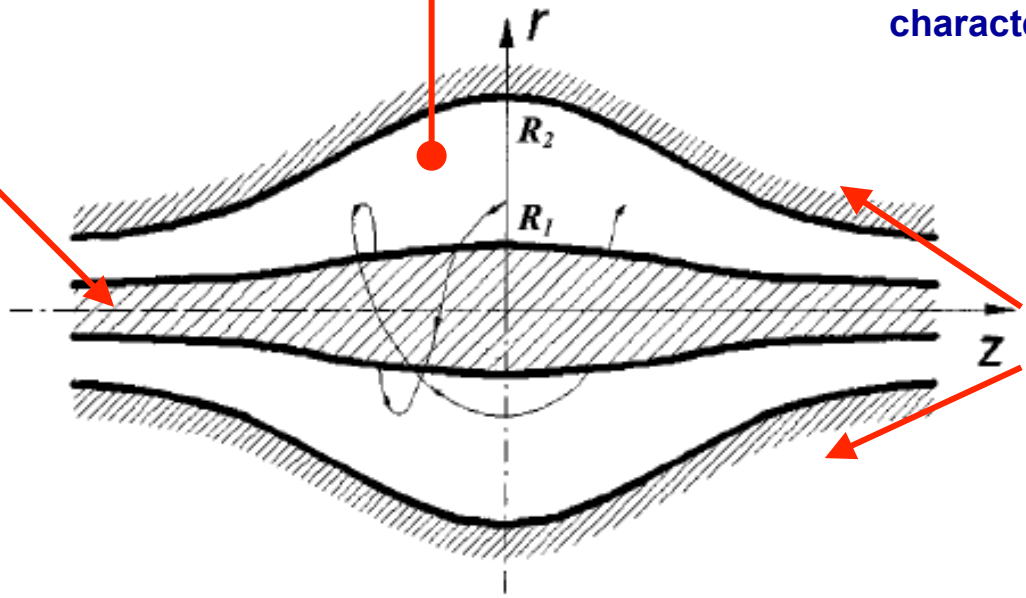
field curvature

Electric Potential

$$U(r.z) = \frac{k}{2}\left(z^2 - \frac{r^2}{2}\right) + \frac{k}{2}(R_m)^2 \ln\left[\frac{r}{R_m}\right] + C$$

characteristic radius

central electrode
(spindle-like, 0V)



outer electrodes
(barrel-like, -5kV)

Figure 1. Equipotentials of the quadro-logarithmic field and an example of a stable ion trajectory

Fourier-Transform Orbitrap Mass Spectrometer

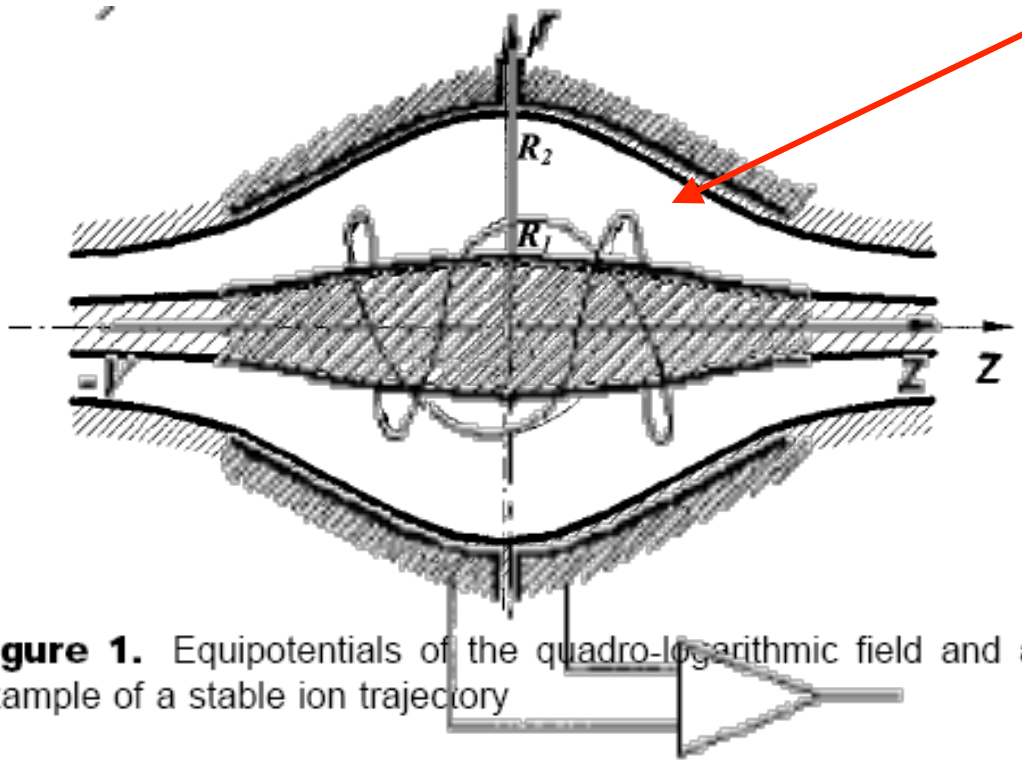


Figure 1. Equipotentials of the quadro-logarithmic field and an example of a stable ion trajectory

ion trajectory in z direction

$$z(t) = z_0 cos(\omega t) + \sqrt{\frac{2E_z}{k}} sin(\omega t)$$

$$\omega = \sqrt{\frac{q}{m} k}$$

Comparison of Important Mass Analyzers

TABLE 3.1. Comparison of Various Types of Mass Analyzers

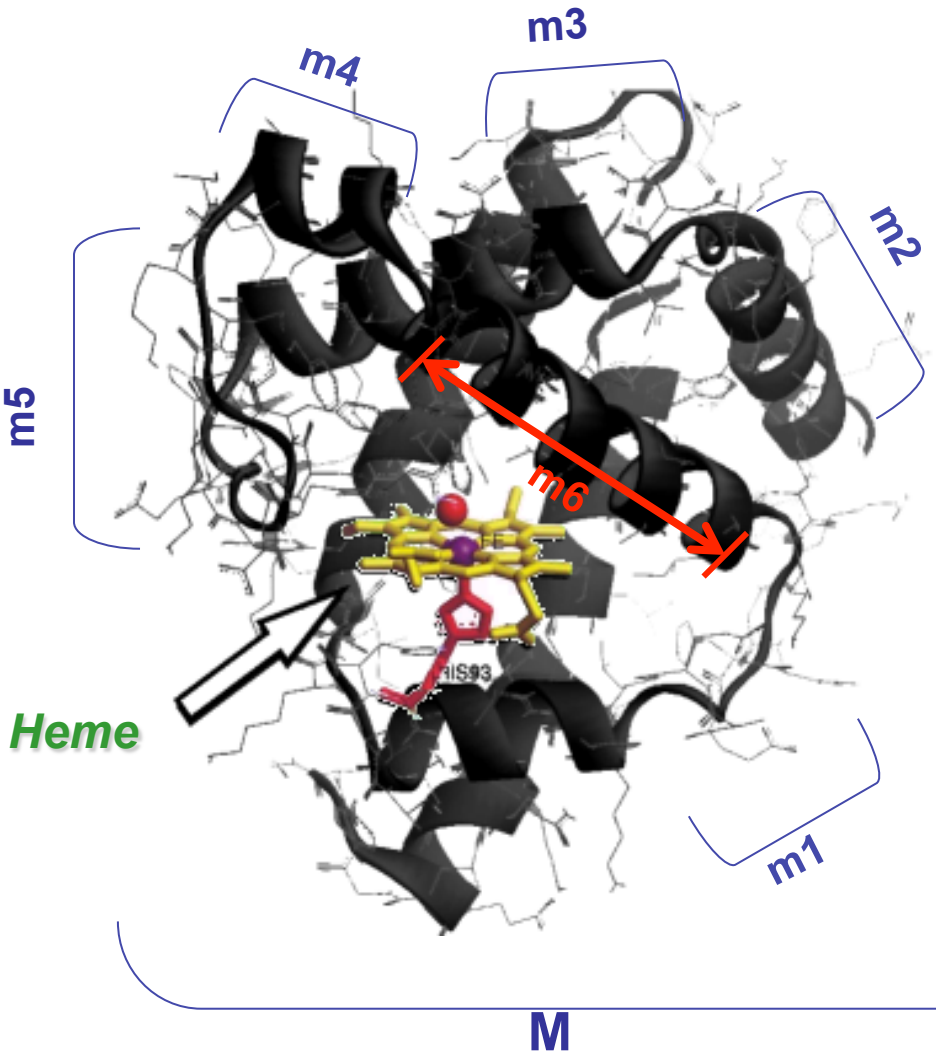
Characteristic	Magnetic	Quadrupole	QIT	LIT	TOF	FT–ICR
Mass range (Da)	15,000	4000	4000	4000	Unlimited	$>10^4$
Resolving power	10^2-10^5	4000	10^3-10^4	10^3-10^4	15,000	$>10^6$
Mass accuracy (PPM)	1–5	100	50–100	50–100	5–50	1–5
Abundance sensitivity	10^6-10^9	10^4-10^6	10^3	10^3-10^5	up to 10^6	10^2-10^5
Speed (Hz)	0.1–20	1–20	1–30	1–300	10^1-10^6	$10^{-2}-10^1$
Efficiency%	<1	<1–95	<1–50	<1–99	1–100	<1–95
Dynamic range	10^9	10^7	10^2-10^5	10^2-10^5	10^2-10^6	10^2-10^5
MS/MS	Excellent	Great	Great	Excellent	Great	Great
LC (CE)/MS	Poor	Excellent	Excellent	Excellent	Good	Good
Cost	$$$$	$	$	$$	$$-$$$	$$$$

Orbitrap

150,000

C. Dass, Fundamentals of Contemporary Mass Spectrometry, John Wiley& Sons, 2007.

Fragmentation of Analytes (for structural identification)



holoMyoglobin

Fragmentation Methods

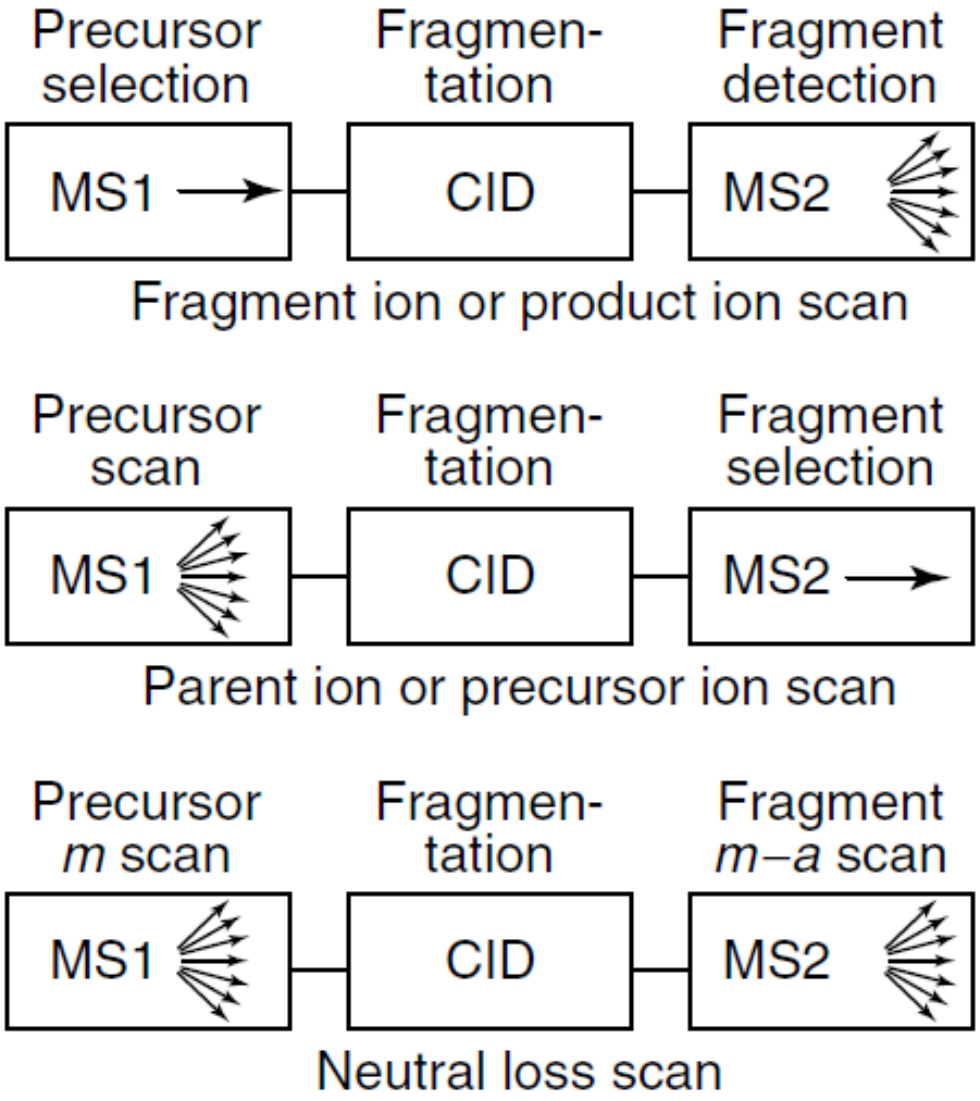
Table 1. General description of different ion activation processes presented

Method	Energy Range	Instruments	Description
PSD	Low	RETOF	Metastable or collision-induced dissociations in flight tube of reflectron time-of-flight instrument
CID	Low	QqQ, IT, QqTOF, QqLIT, FTICR	Collision-induced dissociation by collision of precursor ions with inert target gas molecules in collision cell. Energy range 1–100 eV
	High	Tandem TOF, sectors	Same as above with keV energies
SID	Low	Hybrid (BqQ), QqQ, IT, FTICR	Collisions between precursor ions and solid target surface with or without self-assembled monolayer causing fragmentations as well as other side reactions
	High	Tandem TOF, RETOF	Same as above with precursors of higher translational energies (instrument dependent)
ECD	Low	FTICR	Low-energy beam of electrons resulting in electron capture at protonation (or cationic) site with subsequent fragmentation following radical ion chemistry
ETD (charge neutralization)		**IT**	
IRMPD	Low	IT, FTICR	Continuous-wave low-energy infrared laser activates precursor ions by multiphoton absorption with consequent fragmentation
BIRD	Low	IT, FTICR	Low-energy thermal activation method ideal for calculations of energy thresholds and thermodynamic properties

Orbitrap

L. Sleno, D. A. Volmer, J. Mass Spectrom. 39, 1091 (2004).

Fragmentation Methods



Sulfonation
SO_3: 80 Da

Phosphorylation
HPO_3: 80 Da
H_3PO_4: 98 Da

Fragmentation Technologies

(Bond-breaking process)

energy input energy release

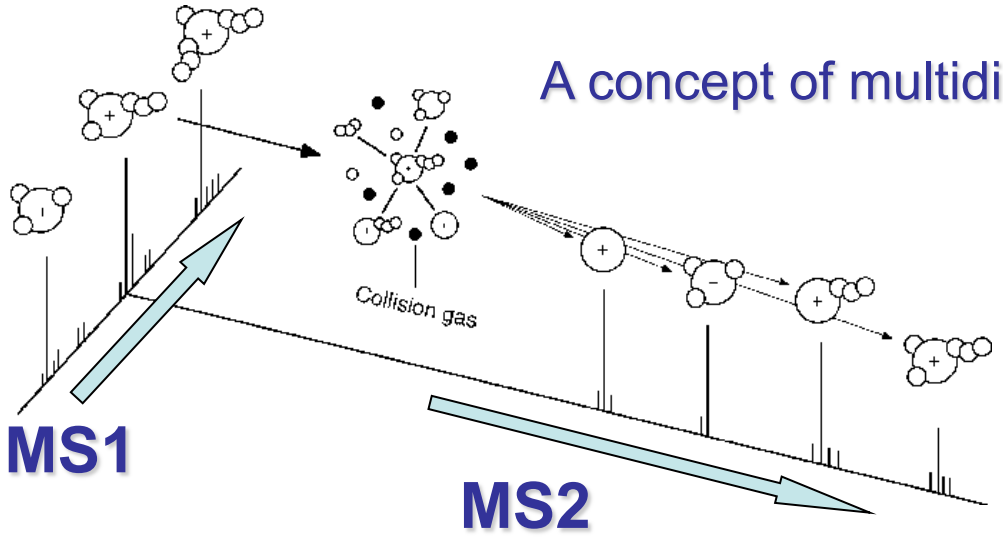
ABCD → **ABCD‡** → **A + B + C + D**

CID (collision-induced dissociation): Ion-neutral collision

IRMPD (infrared multiphoton dissociation): Laser heating

ECD (electron-capture dissociation): Charge recombination

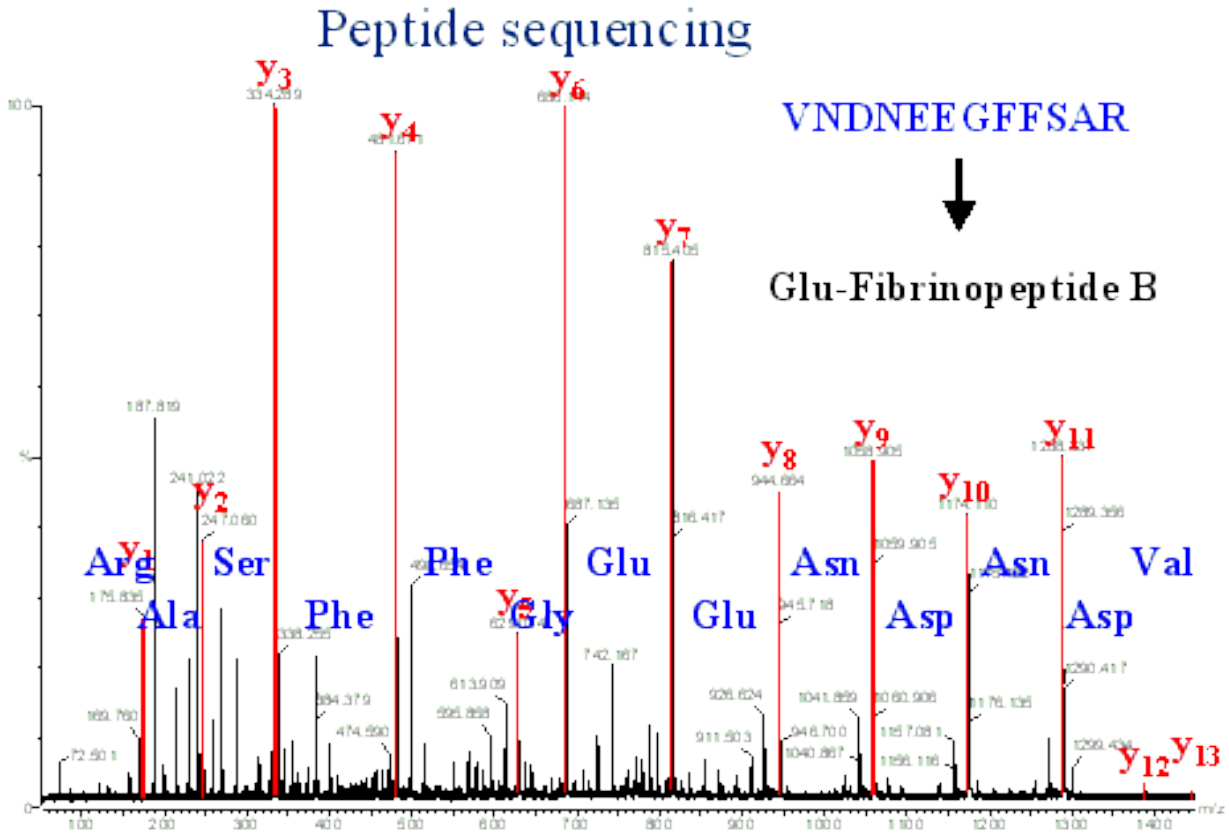
ETD (electron-transfer dissociation): Charge recombination



A concept of multidimensional mapping (MS^n or MS/MS)

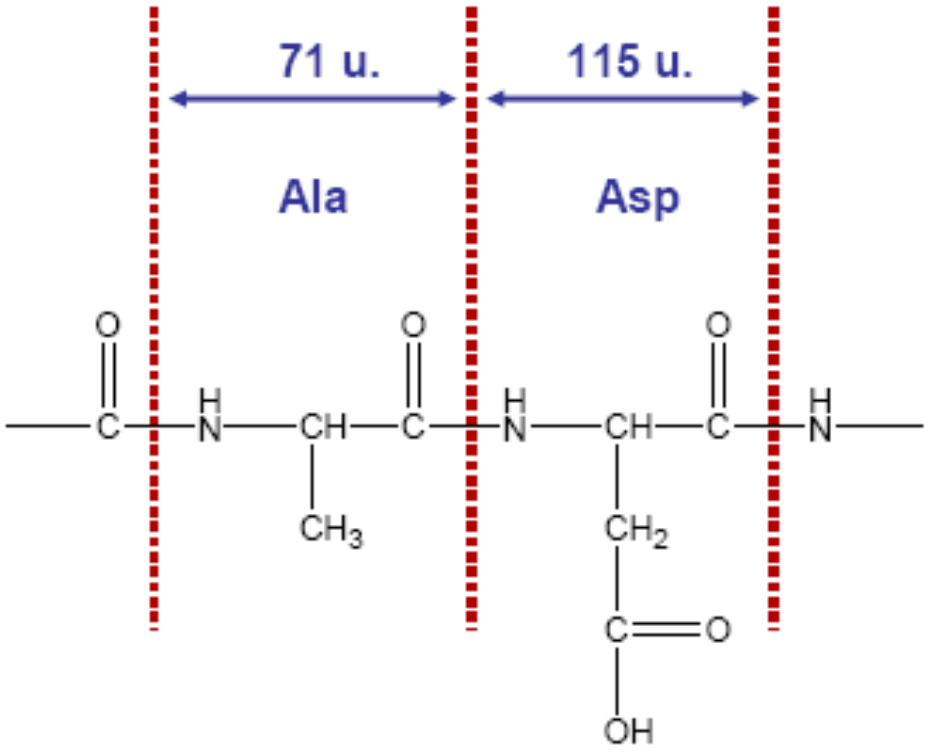
Peptide mass fingerprinting

Peptide Mass Fingerprinting (PMF) is a technique used to identify proteins by matching their constituent fragment masses (peptide masses) to the theoretical peptide masses generated from a protein or DNA database. This technique does well with 2D gel spots where the protein purity is high. PMF protein identification can run into difficulties with complex mixtures of proteins



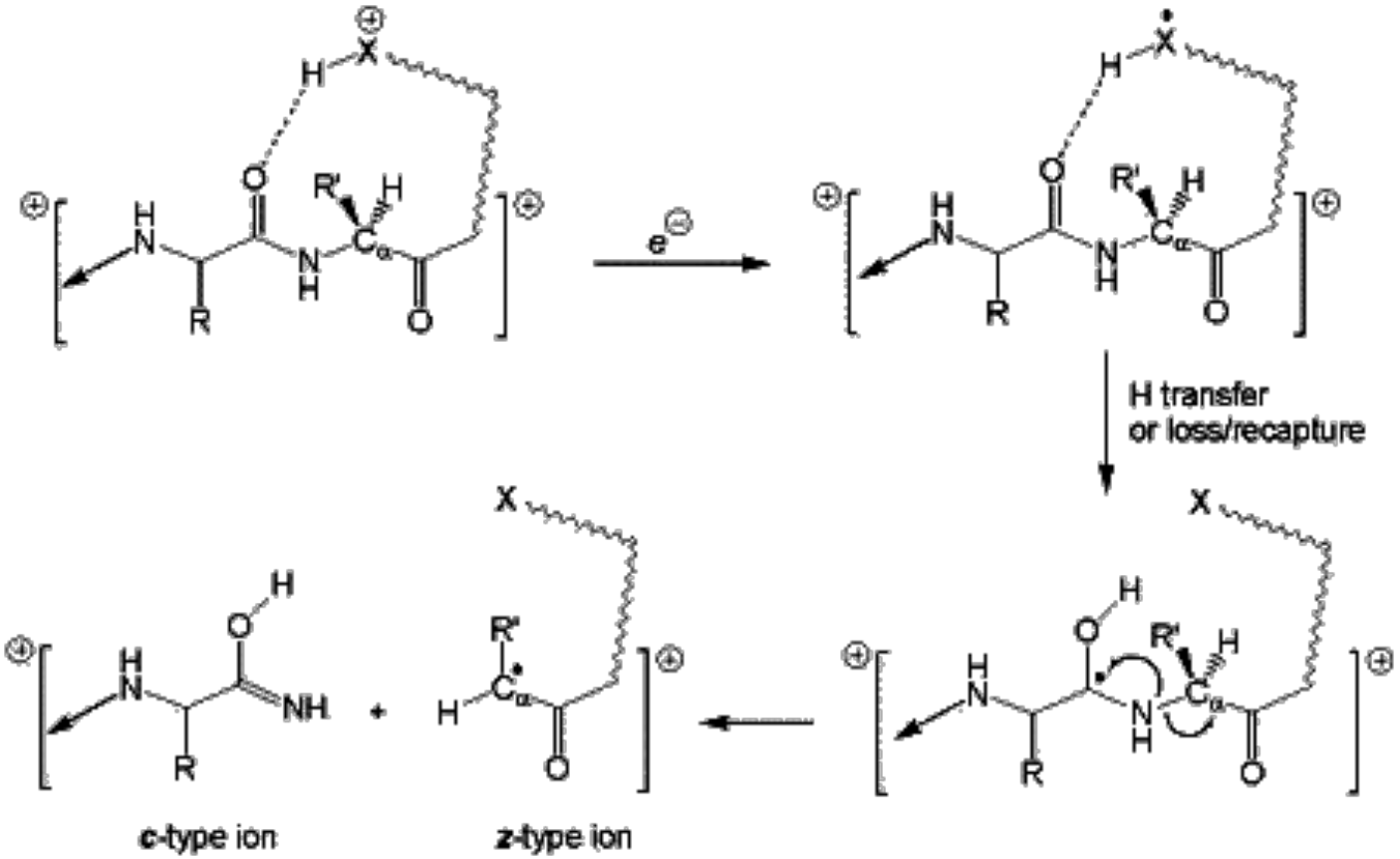
Dr H.M. Davey
Cledwyn Building
Institute of Biological Sciences
University of Wales

Peptide Sequencing



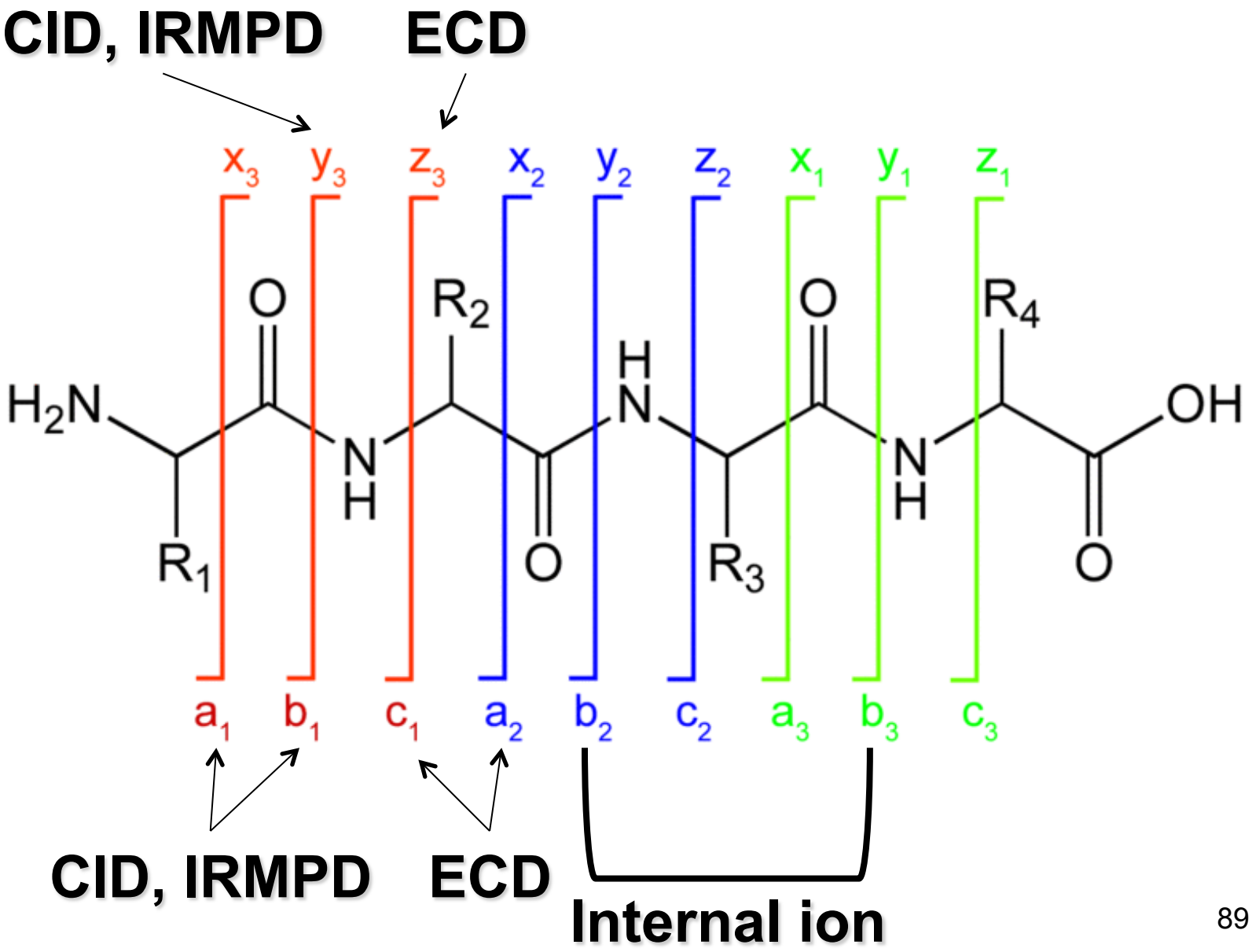
amino acid			mass
Alanine	ALA	A	71.09
Arginine	ARG	R	156.19
Aspartic Acid	ASP	D	115.09
Asparagine	ASN	N	114.11
Cysteine	CYS	C	103.15
Glutamic Acid	GLU	E	129.12
Glutamine	GLN	Q	128.14
Glycine	GLY	G	57.05
Histidine	HIS	H	137.14
Isoleucine	ILE	I	113.16
Leucine	LEU	L	113.16
Lysine	LYS	K	128.17
Methionine	MET	M	131.19
Phenylalanine	PHE	F	147.18
Proline	PRO	P	97.12
Serine	SER	S	87.08
Threonine	THR	T	101.11
Tryptophan	TRP	W	186.12
Tyrosine	TYR	Y	163.18
Valine	VAL	V	99.14

Electron-capture dissociation (ECD)

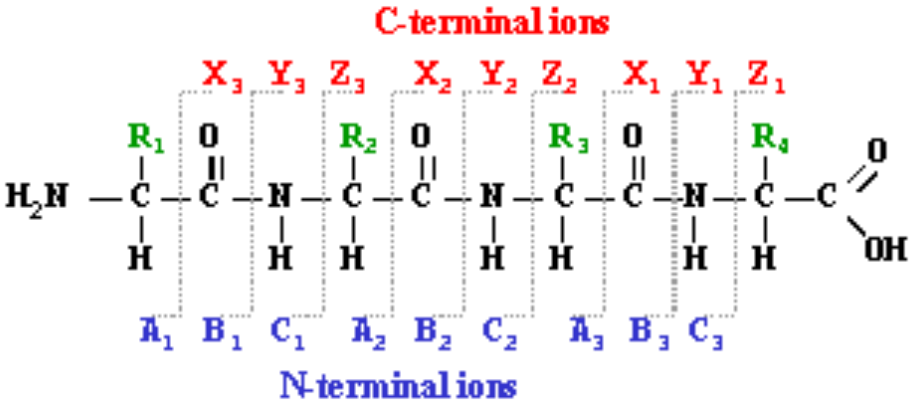


Scheme 1. The current ECD mechanism for H atom transfer and dissociation in internally-solvated peptide ions.

Cleavage Sites of Peptides



Site-specific cleavage on peptides: a/z, b/y, c/x fragmentations



P-A-F-D-S-I-M-A-E-T-L-K
(protonated mass 1410.6)

mass$^+$	b-ions	y-ions	mass$^+$
88.1	S	PAFDSIMAETLK	1323.6
185.2	SP	AFDSIMAETLK	1226.4
256.3	SPA	FDSIMAETLK	1155.4
403.5	SPAF	DSIMAETLK	1008.2
518.5	SPAFD	SIMAETLK	893.1
605.6	SPAFDS	IMAETLK	806.0
718.8	SPAFDSI	MAETLK	692.3
850.0	SPAFDSIM	AETLK	561.7
921.1	SPAFDSIMA	ETLK	490.6
1050.2	SPAFDSIMAE	TLK	361.5
1151.3	SPAFDSIMAET	LK	260.4
1264.4	SPAFDSIMAETL	K	147.2

Techniques for Protein Sequencing

Bottom-Up

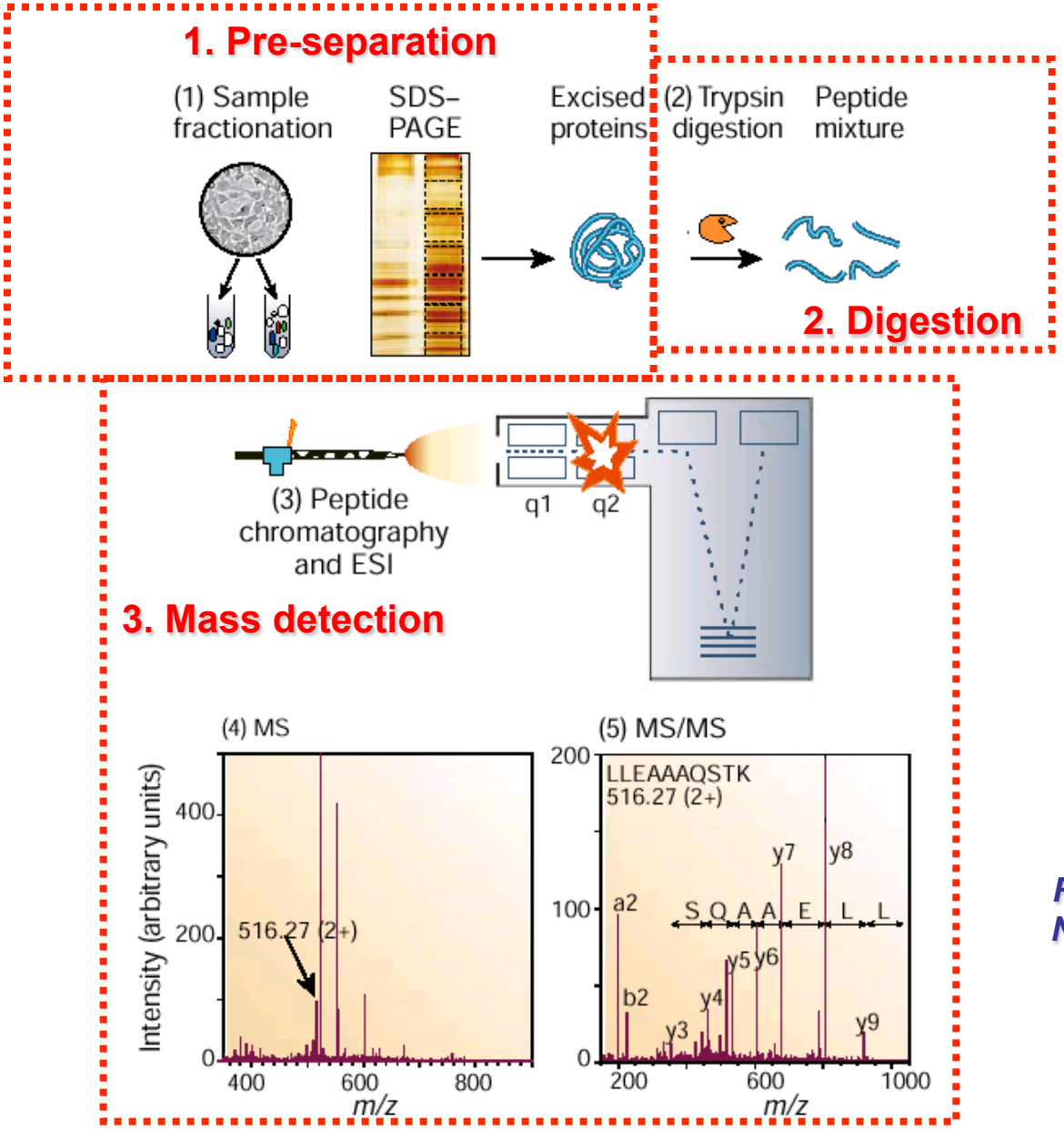
This term refers to approaches that have been developed for the identification of proteins and the in-depth characterization of their structure. The term Bottom-Up reflects the **reconstruction of the primary structure of the proteins from the little pieces of sequences of the peptides** that could either be identified in databases or derived from the analysis of their mass spectra. Bottom-up approaches are often applied on protein mixtures in comparative proteomics.

Top-Down

This term refers to approaches that **attempt to determine the structure of the protein directly on the protein itself without breaking it into pieces by digestion**. The Top-Down approach makes use of mass spectrometers capable of isolating ions of the protein and breaking them into fragments of interpretable size that bear sequence information. The Top-Down approach relies also heavily on specific database-search engines to facilitate the interpretation.

Bottom-Up Proteomics

Build up the protein model from peptide fragments.



R. Aebersold, M. Mann, Nautre, 422, 198 (2003).

Top-Down Proteomics

Break down the protein structure starting from an intact molecule.

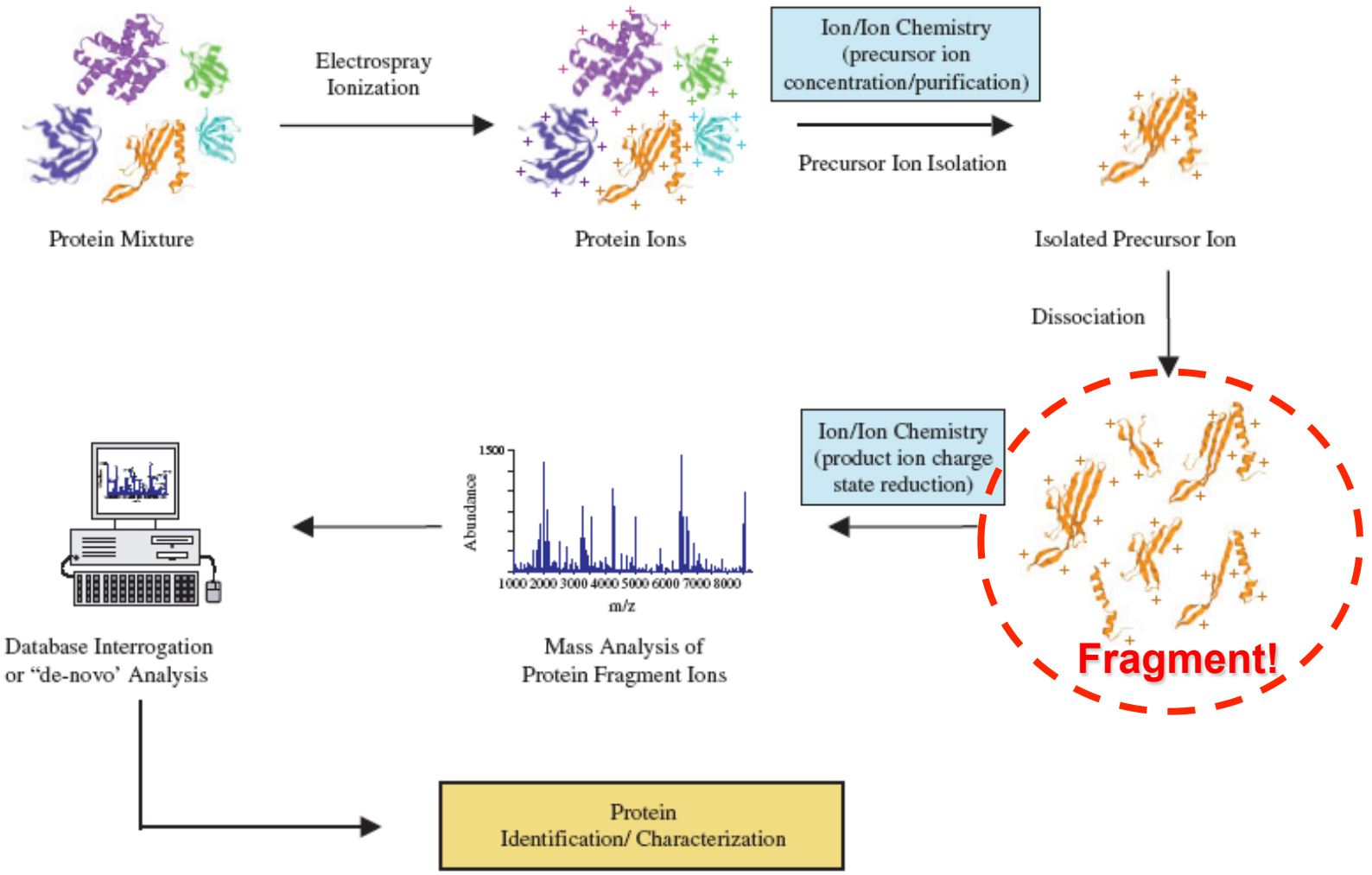


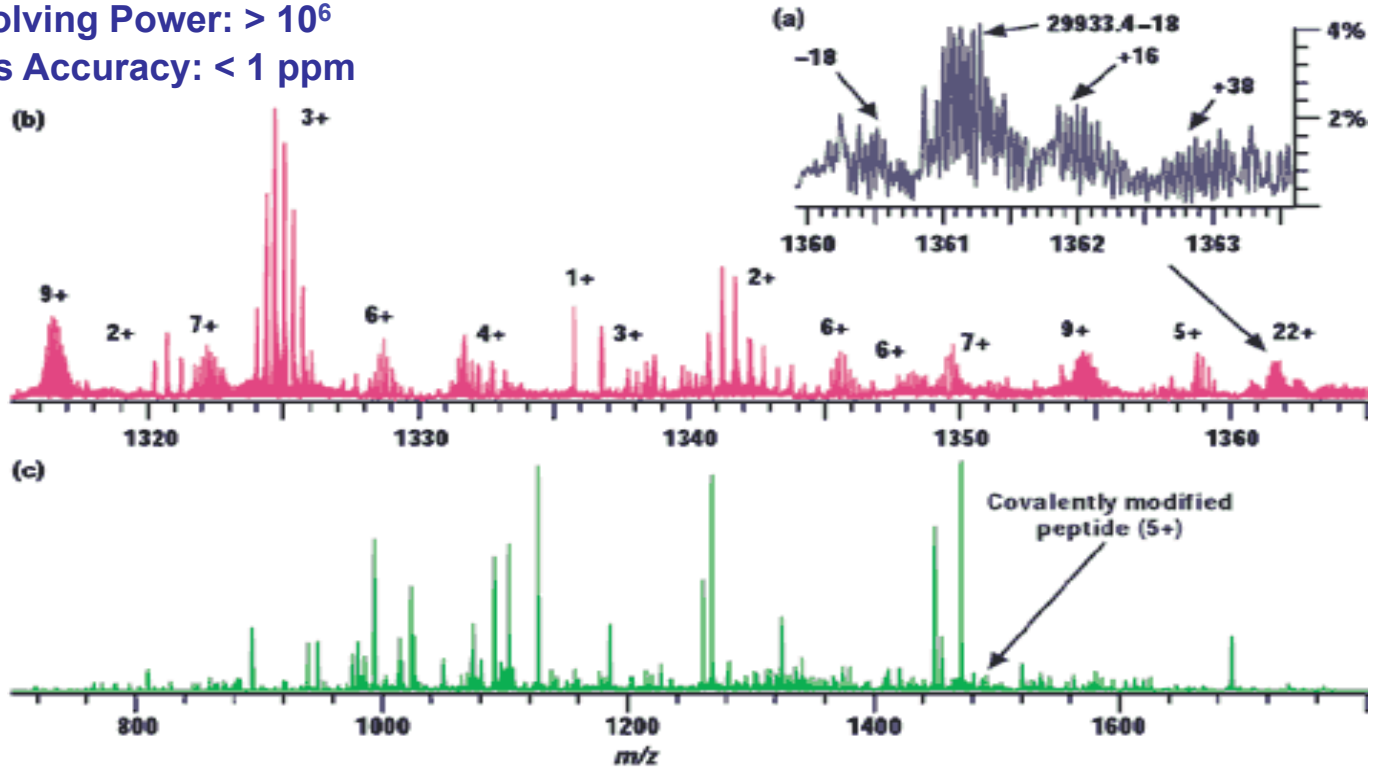
Plate 1. Schematic diagram of a typical top down protein characterization experiment. The light blue shaded boxes indicate where gas-phase ion–ion chemistries may be employed in top down approaches (see text).

WHEN

- *Identification of unknown molecules*
- *Imaging mass spectrometry*
- *Discussions and perspectives*

Advantage of High Resolution MS

Resolving Power: > 10^6
Mass Accuracy: < 1 ppm



(a, b) Two m/z scale-expanded segments from (c) an ESI FT-ICR broadband mass spectrum of a GluC digest of a 191-kDa protein.

The charge state of each peptide in (a) and (b) was determined from the reciprocal of the spacing between adjacent peaks in each isotopic distribution, of which there were 824. From the single broadband spectral data in (c), 581 individual peptides could be identified, along with the site of a single amino acid chemical modification.

A. G. Marshall, C. L.Hendrickson, Stone D.-H. Shi, Anal. Chem. 74(9), 252 (2002).

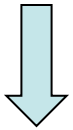
Determining small molecule structure

Field	Res. (Mil.)	Acc. (ppm)
7T	>1	<1
9.4T	>1.5	<0.5
12T	>2	<0.3
15T	>2.5	<0.25

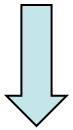
Bruker Daltonics' catalog

Measure the precise m/z,
FT-ICR (9.4T) mass accuracy < 0.5 ppm,
Resolving power > 1.5 M

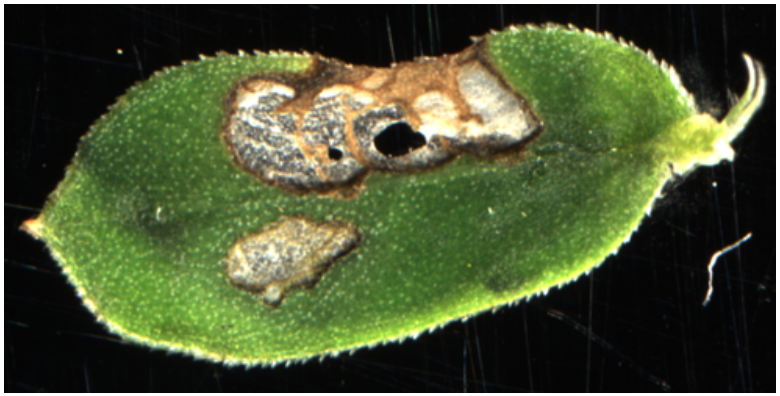
For M/Z = 1000, ΔM/Z < 0.001

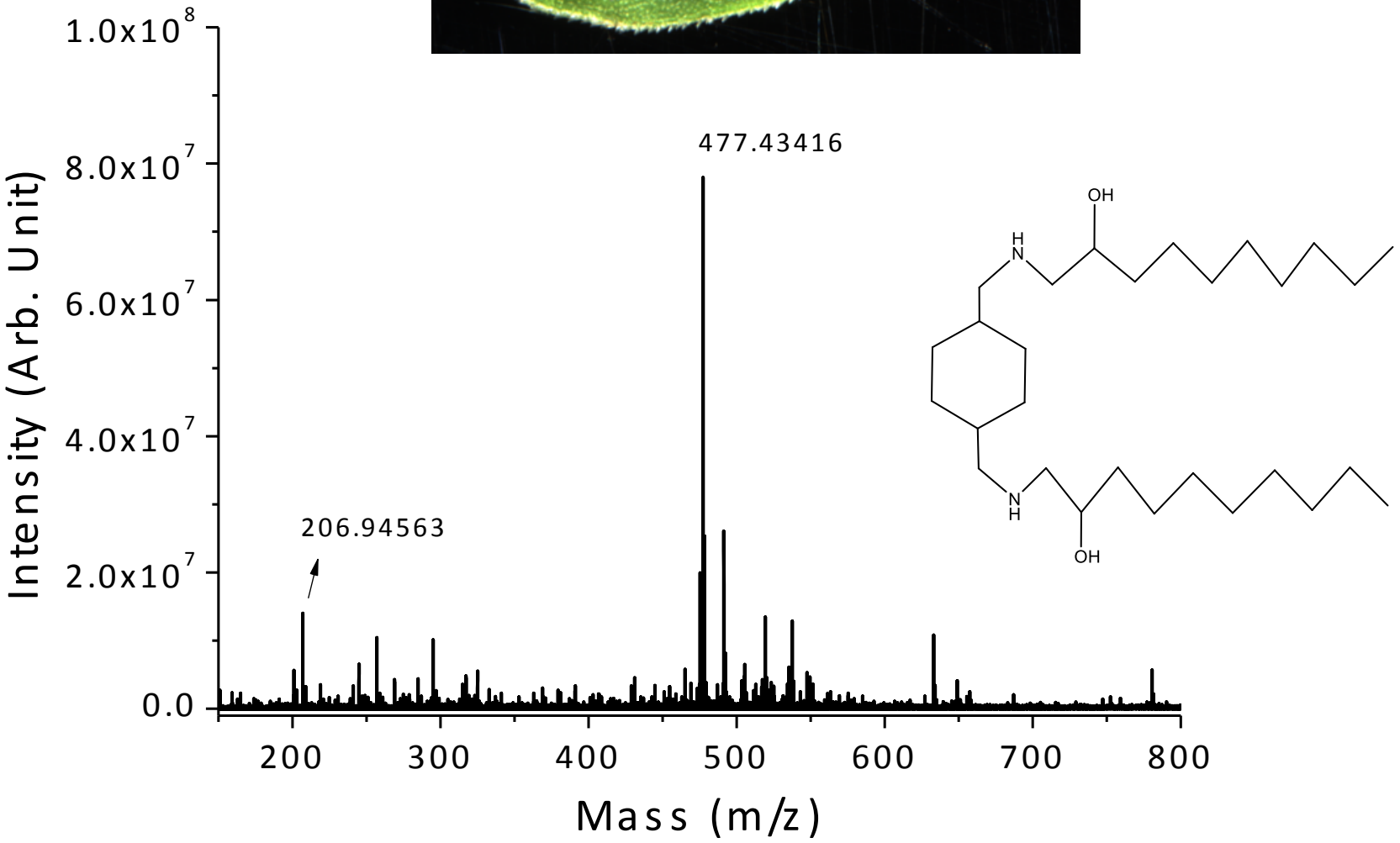


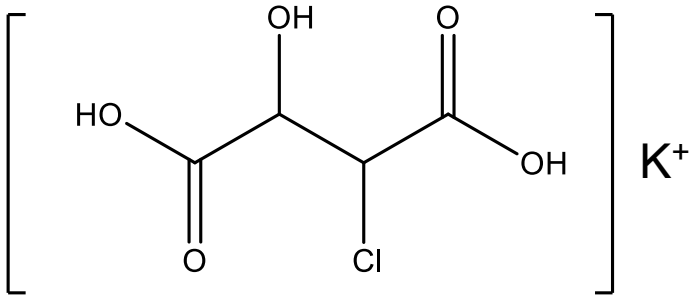
Predict chemical formula
ΔM/Z, isotope pattern, π+ring, C/H ratio



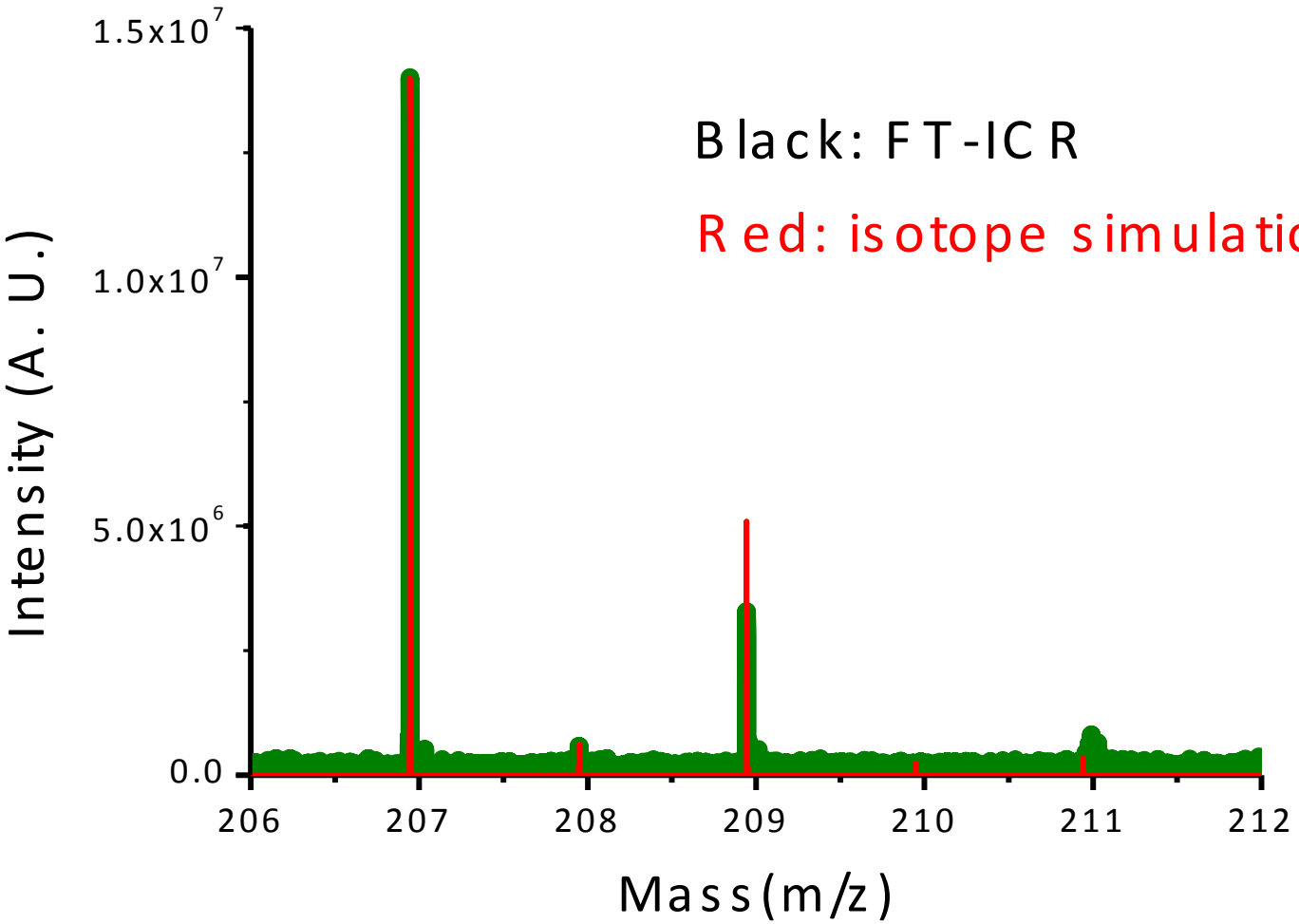
Search structure on SciFinder
Search by chemical formula




1.0x10^8
8.0x10^7
6.0x10^7
4.0x10^7
2.0x10^7
0.0
Intensity (Arb. Unit)
477.43416
206.94563
200
300
400
500
600
700
800
Mass (m/z)
OH
H
N
N
H
OH



2-chloro-3-hydroxy-butanedioic acid

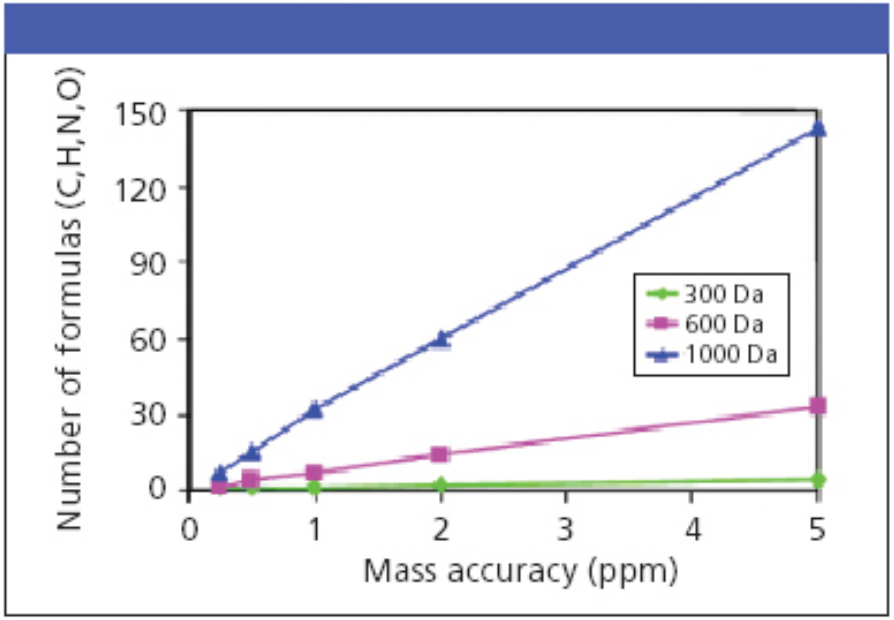


Measuring the precise m/z

For “unambiguous characterization”:

M/Z	Mass acc.
118	34 ppm
750	0.018ppm

Author’s guideline of the JASMS, (March 2004)



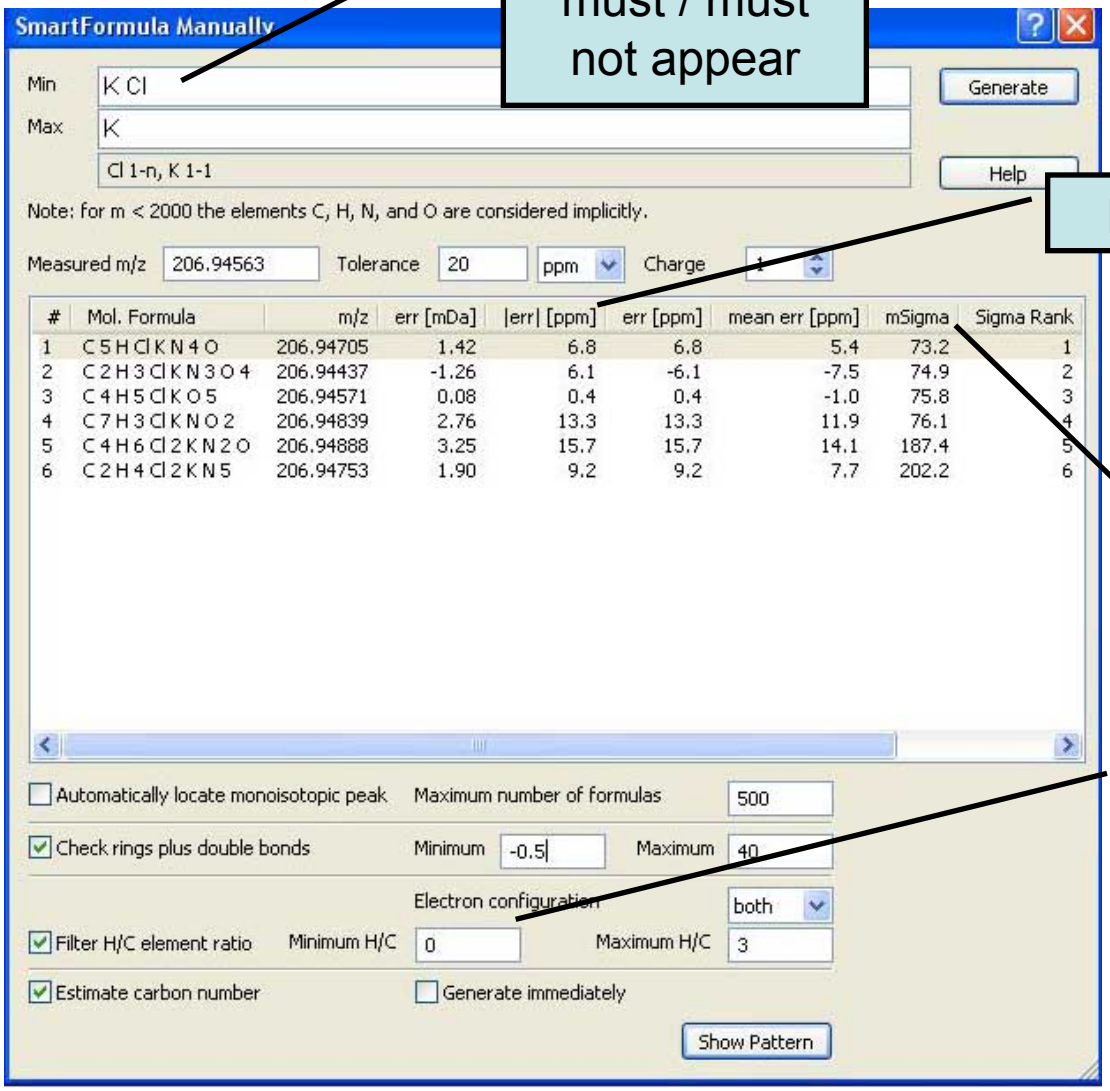
T.L. Quenzer, et. Al., Automated accurate mass analysis using FTICR mass spectrometry, Proceedings of the 50th Annual Conference on Mass Spectrometry and Allied Topics, Orlando, Florida, 2002

Table 1: A comparison of leading higher resolution mass spectrometers (adapted from reference 1).

	Resolution (FWHM)	Mass range (*m/z*)	Mass accuracy (ppm)	Price ($, typical range comparison)
TOF			2–5 typical	200–250K
Waters LCT Premier	10000	18000		
Agilent LC/MSD TOF	10000	7000		
Bruker MicroTOF	10000	3000		
Q-TOF			Same as TOF	300–700K (450K typical)
Waters QTOF Ultima	17500	32000		
Waters QTOF Micro	5000	20000		
MDS Sciex Qstar XL	10000	40000 (TOF) 20000 (Q)		
Bruker BioTOF	20000	10000 (TOF)		
ICR (FT–MS)				500K–1.4M
Bruker Apex IV	100000	66000	<1	
Ion Spec	1300000	18000	1	
Thermo LTQ FT	500000	2000	2	

Debating resolution and mass accuracy, Micheal P. Balogh, 2004

Predict chemical formula



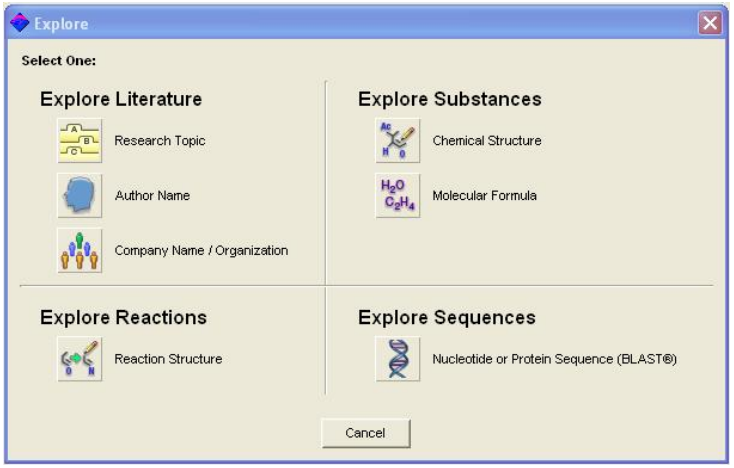
Atoms that must / must not appear

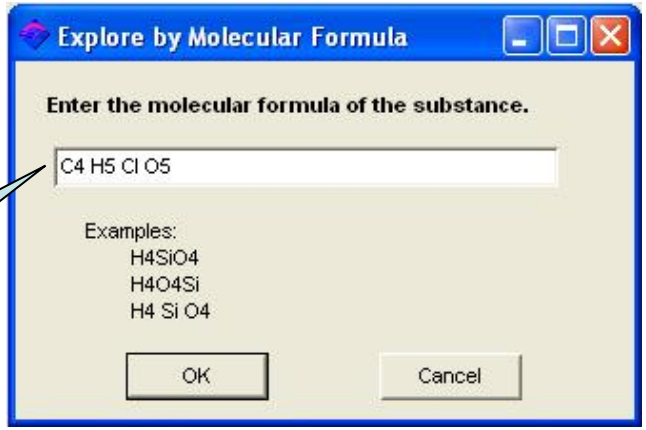
M/Z bias

Isotope pattern similarity

Feature of the molecule. Ex.
Cabohydrate ~1:2
Protein 1:1.4~1.5
DNA ~1:1.2

Search structure on SciFinder





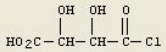
Note that charge carrier (K^+) was removed

SciFinder

File Edit View Task Tools Help

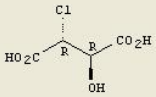
New Task | Back | Forward | Print | Save As | Full Text | Prefs | Combine | History | Contact | Internet | Panorama | Help | Exit

859980-78-2



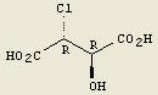
~1 Reference
REGISTRY

742046-86-2



No References
REGISTRY

165877-67-8



~1 Reference
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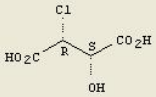
112335-64-5



~1 Reference
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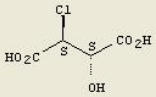
74841-95-5



~2 References
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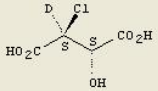
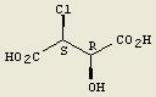
74804-17-4



~1 Reference
REGISTRY

21788-47-6



~4 References
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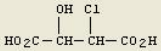
19071-25-1



~12 References
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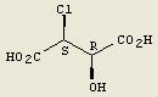
7403-74-9



~2 References
REGISTRY

Get References | Get Reactions | Analyze/Refine | Back

Substances 1-9 of 9

Imaging Mass Spectrometry

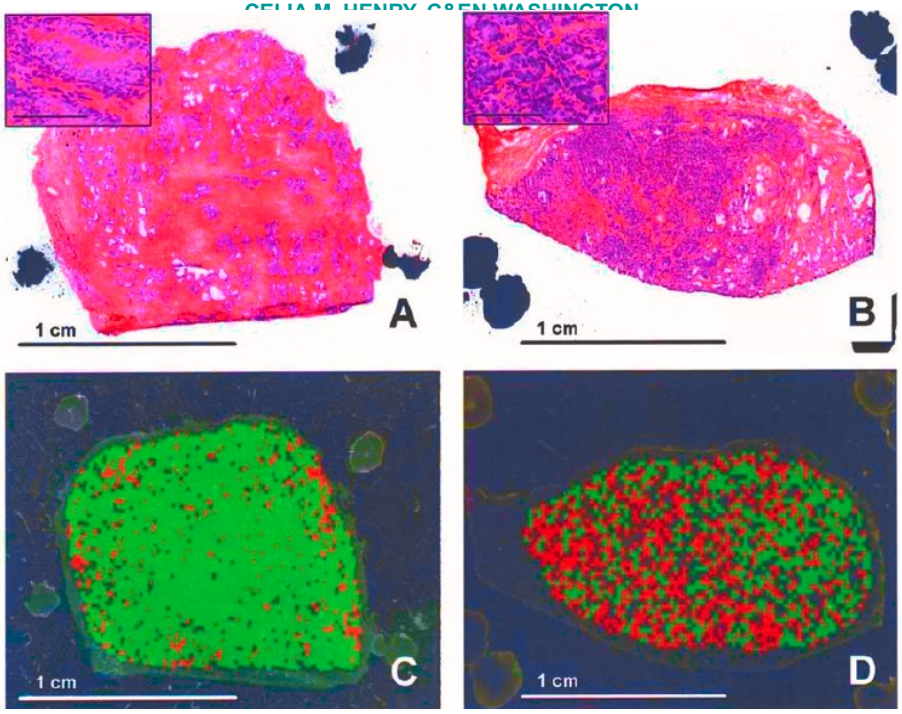
making mass spectrometer the chemical microscope

CHEMICAL & Engineering News
Science & Technology
November 15, 2004
Volume 82, Number 46
pp. 33-35

DRAWING WITH MASS SPEC

Mass spectrometry is emerging as a tool to image biological samples from single cells to brain slices

CELIA M. HENRY, C&EN WASHINGTON



Schwamborn K. et al, Int. J. Mol. Med. (2007), 20, 155-159.

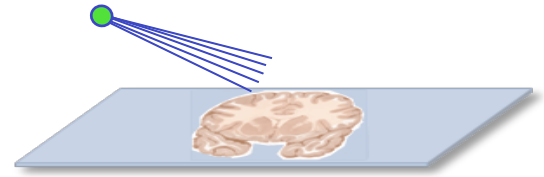
If a picture is wort al information? Mass spectrometric imaging rovide the "colors." It takes familiar mass sp roscope. So, given a two-dimensional sampl masses are located. Especially in biologica sual inspection long associated with fields s

These pictures are n or the sample, and acquiring mass spectr stribution of specific components can be re rum at each spot, or "pixel." Multiple picture set of spectra. Using smaller, more tightly f xels means that the image takes longer to c

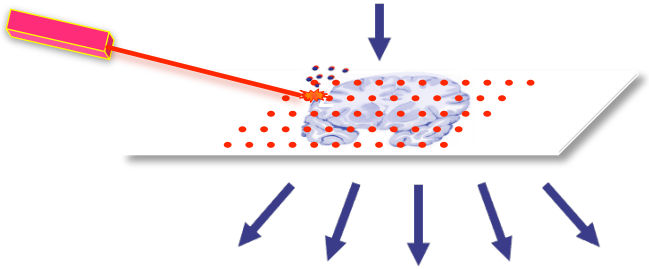
Most mass spectr n the sample: matrix-assisted laser desorpti IMS). In MALDI, the sample is covered wit o desorb and ionize components. In SIMS, k molecules from the surface and ionize them. The two methods are complementary: MALDI works well for relatively large molecules such as peptides and proteins, whereas SIMS is better for small molecules.

Basic Approach of MALDI Imaging MS for Tissue Analysis

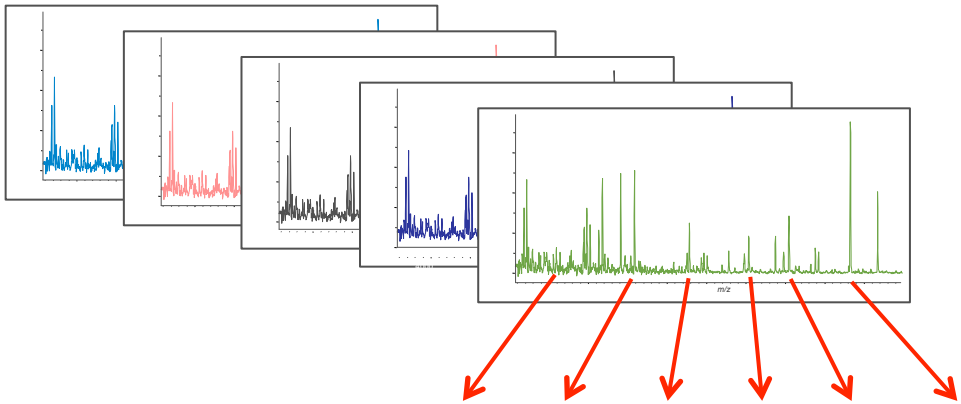
Prof. Richard M. Caprioli
Vanderbilt University
Tennessee, USA



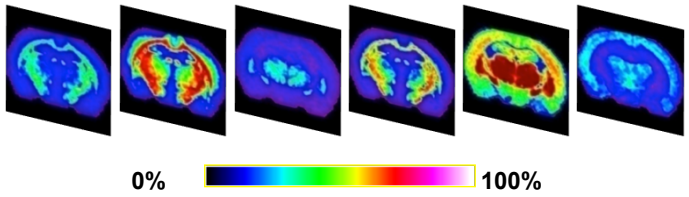
Apply matrix to tissue section



Laser ablation of array of x,y coordinate positions (pixels)



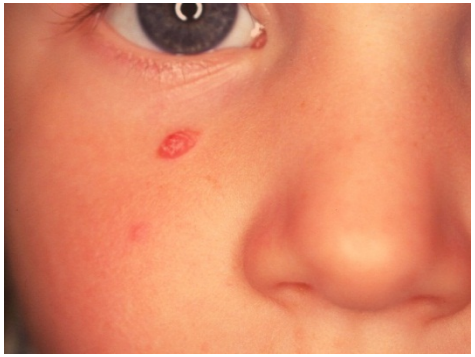
Mass spectrum from each pixel

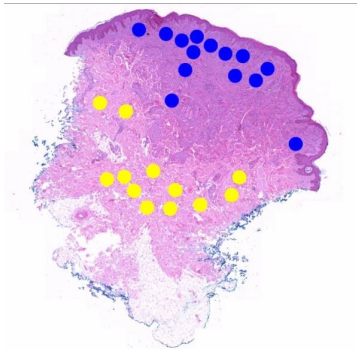


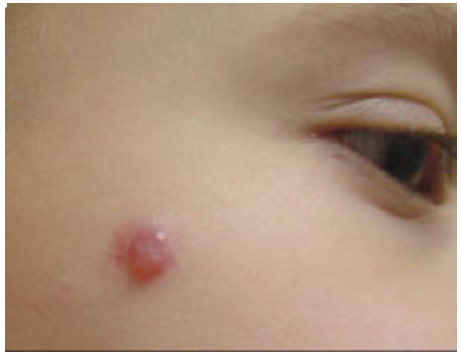
Images at single *m/z* values integrated over all pixels

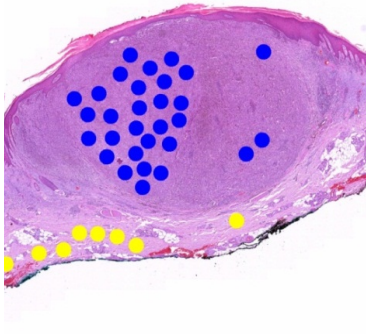
MS Analysis of Spitzoid Lesions in FFPE Biopsies

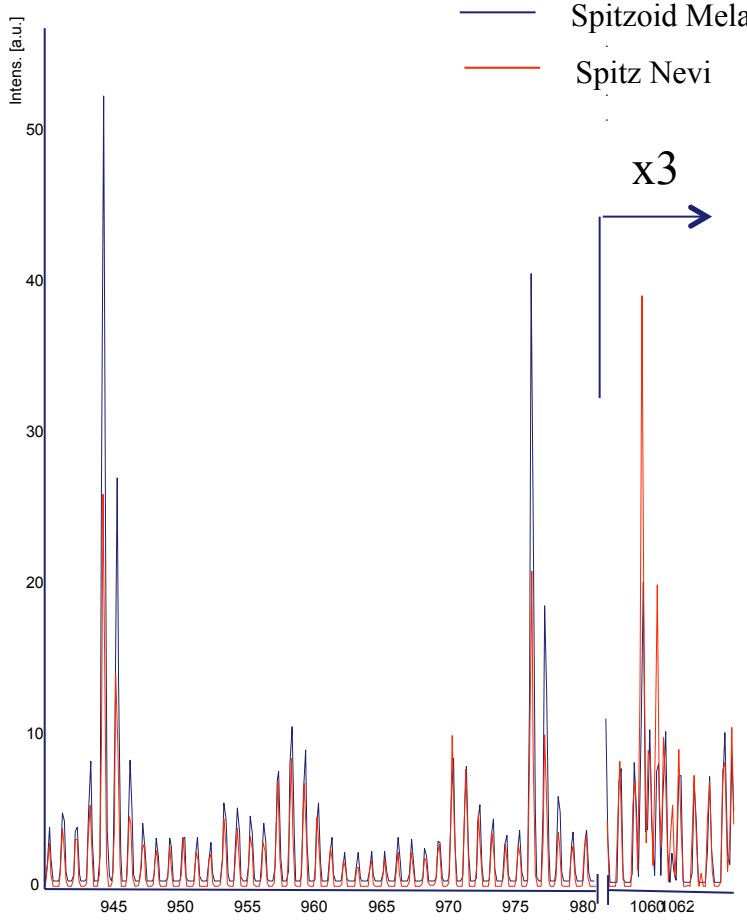
Prof. Richard M. Caprioli
Vanderbilt University
Tennessee, USA











Erin Seeley, Rossitza Lazova (Yale)

Prof. Richard M. Caprioli
Vanderbilt University
Tennessee, USA

Classification of Spitzoid Lesions

Training set	# Patients	Classification Accuracy (%)
Spitz nevi (SN)	26	100
Spitzoid Malignant Melanoma (SMM)	25	96

Validation (test) set	# Patients	Classification Accuracy (%)
Spitz nevi (SN)	30	97
Spitzoid Malignant Melanoma (SMM)	29	90

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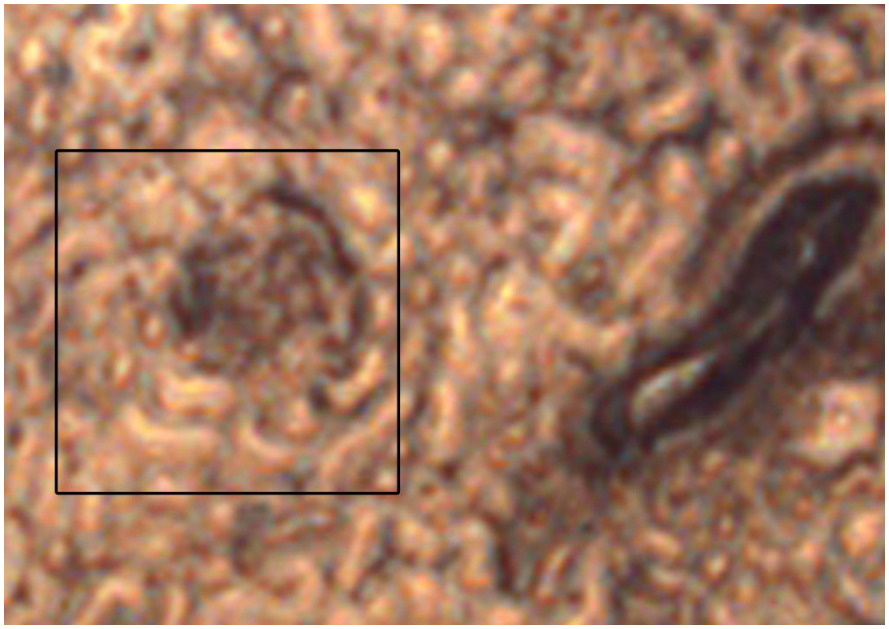
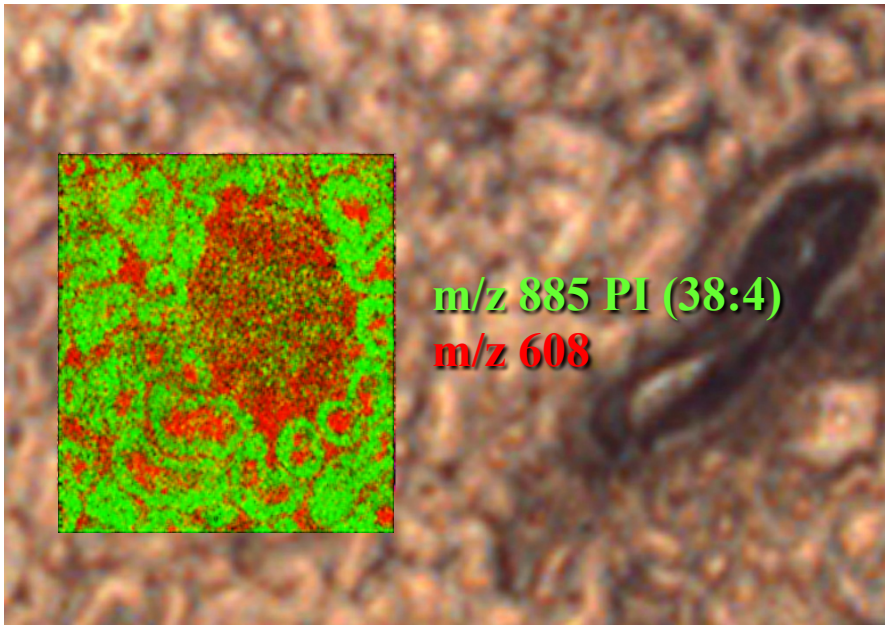
Vanderbilt University
Tennessee, USA

Ion Images of Human Kidney Cortex

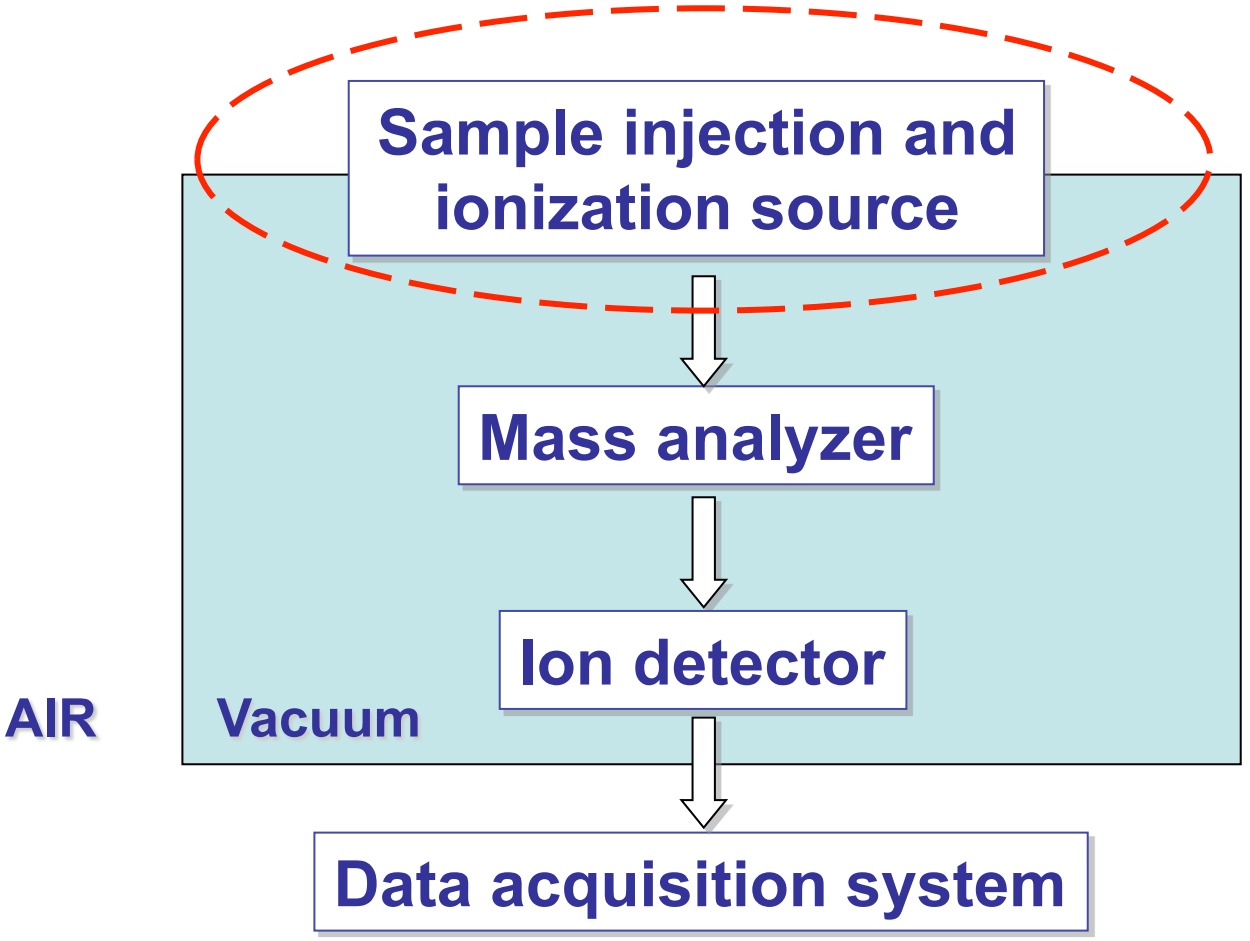
Resolution: 1 μm laser beam, 2 μm pitch
25 shots/pixel, transmission geometry
matrix sublimed DAN





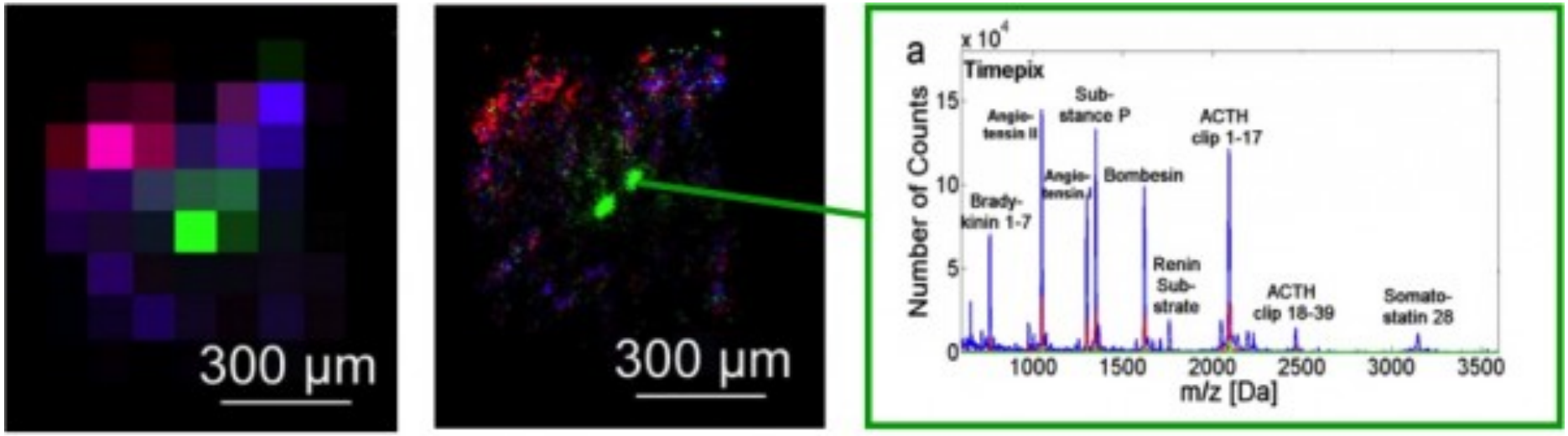
m/z 750 PE (18:0p/20:4)
m/z 1052 Hex-Sulfo-Hex-Cer-(d16:1/26:0)
m/z 906 SulfoHex-Cer (t18:0/24:1)

General Configuration of Mass Spectrometer



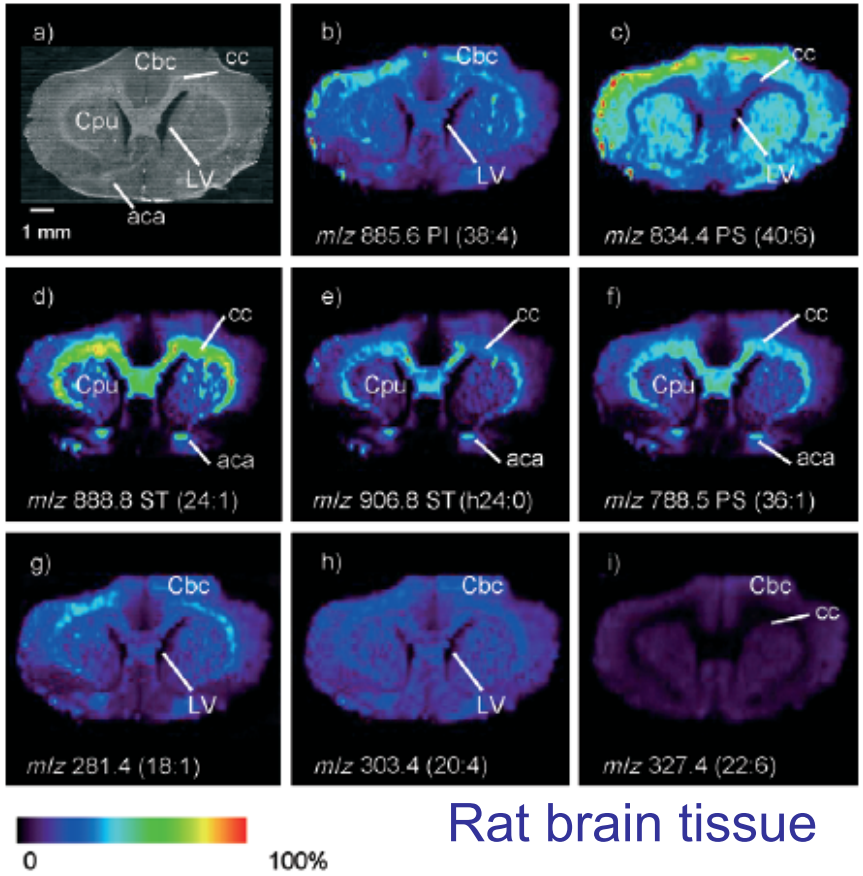
Available Imaging Techniques

- Millimeter scale imaging: DESI
- Micron scale imaging: MALDI
- Sub-micron scale imaging: SIMS



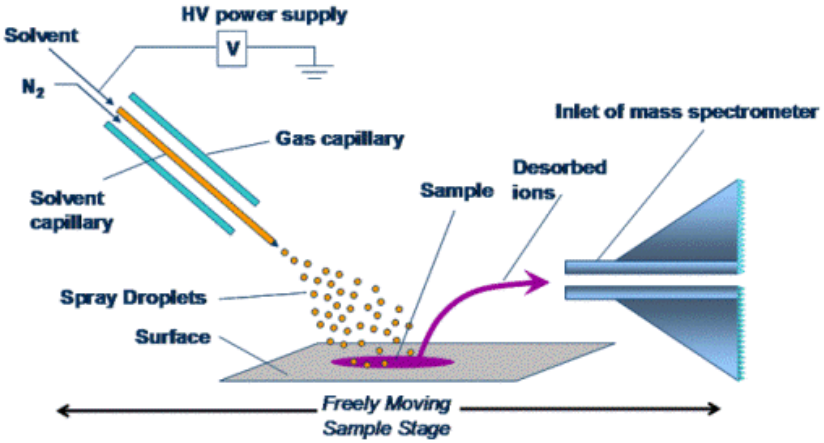
OMICS2IMAGE

Imaging mass spectrometry in millimeter resolution



Rat brain tissue

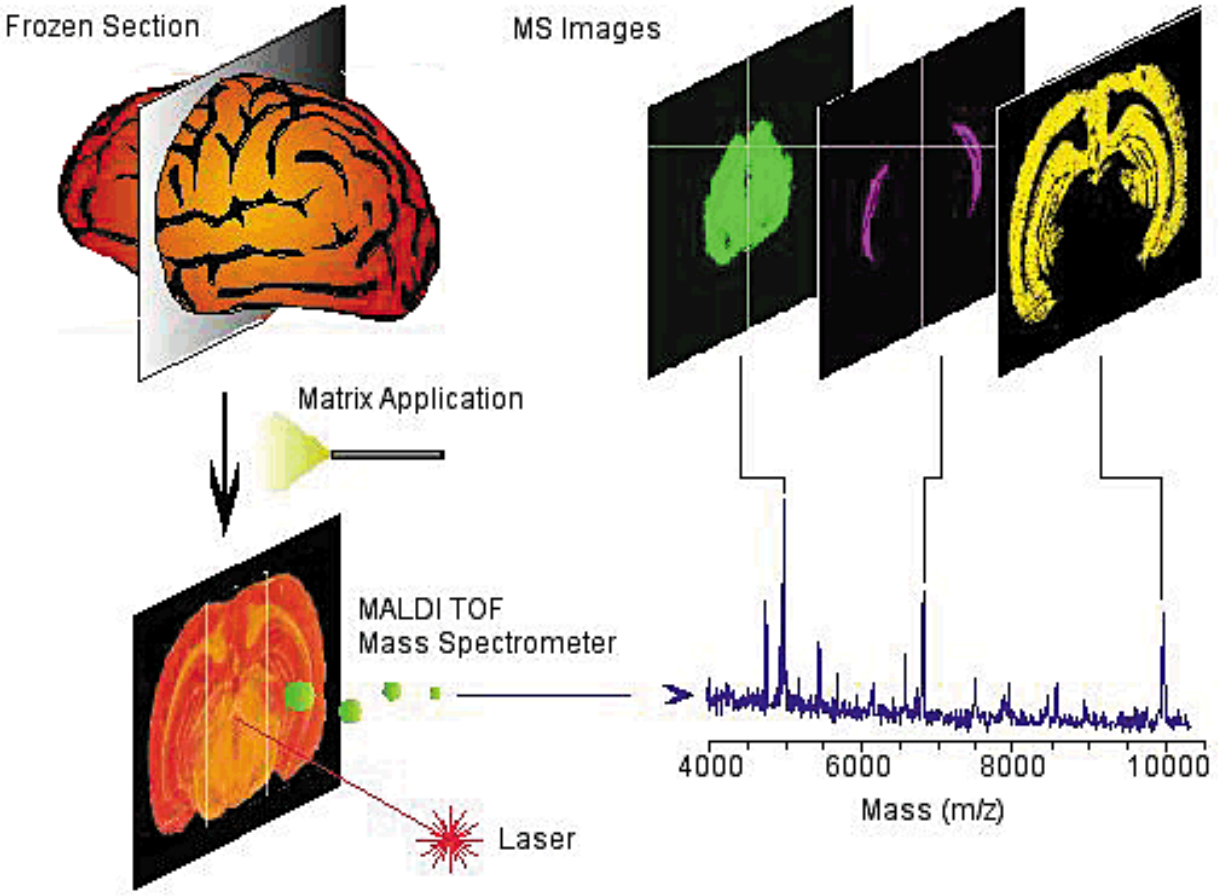
Figure 2. Selected molecular ion $[M-H]^-$ images of specific lipids from analysis of a 13×10 mm² area of rat brain tissue section. a) Optical image of the coronal section of the rat brain prior to analysis. cc = corpus callosum; CPu = striatum; Cbc = cerebral cortex; LV = lateral ventricle; aca = anterior part of anterior commissure. b–i) Ion images of PI (38:4; b), PS (40:6; c), ST (24:1; d), ST (h24:1; e), PS (36:1; f), oleate (18:1; g), arachidonate (20:4; h), and docosahexaenoate (22:6; i).



Prosolia Inc.

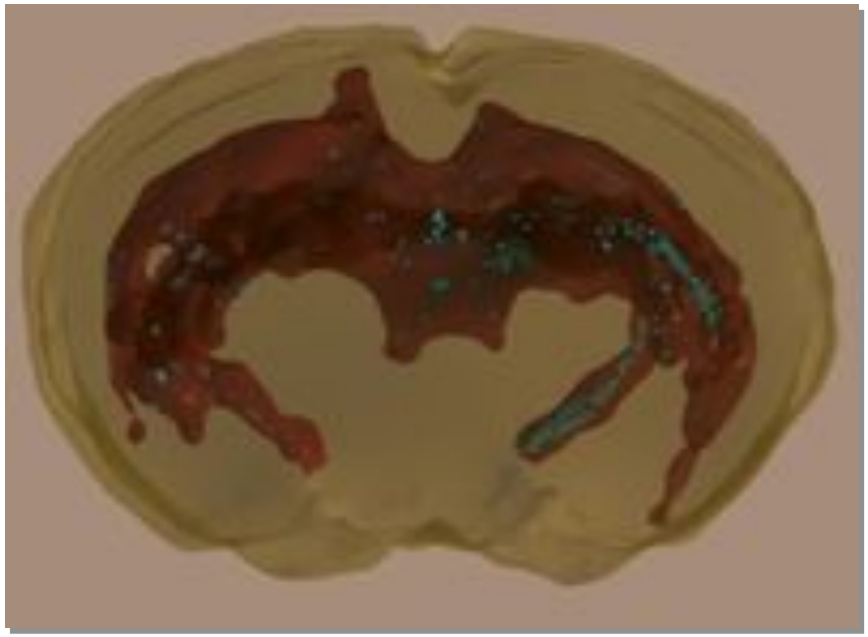
J. M. Wiseman, D. R. Ifa, Q. Song, R. G. Cooks, *Angew. Chem. Int. Ed.* 45, 7188-7192 (2006).

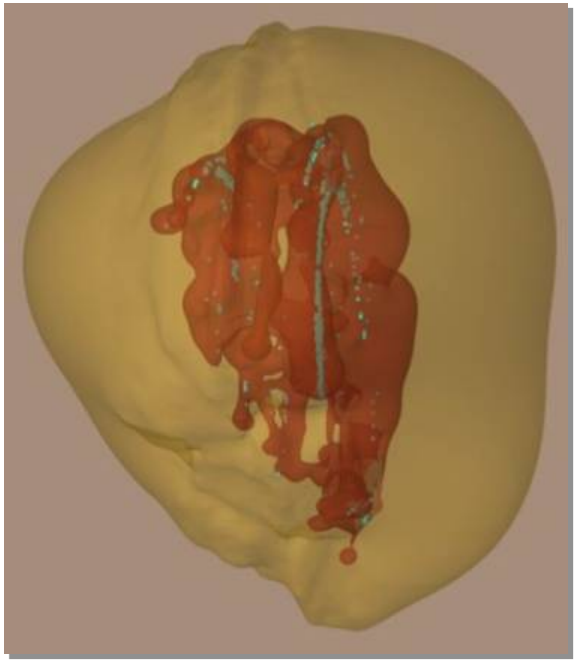
Imaging mass spectrometry in micrometer resolution



M. Stoeckli, P. Chaurand, D. E. Hallahan, R. M. Caprioli, *Nature medicine* 7(4), 493-496 (2001).

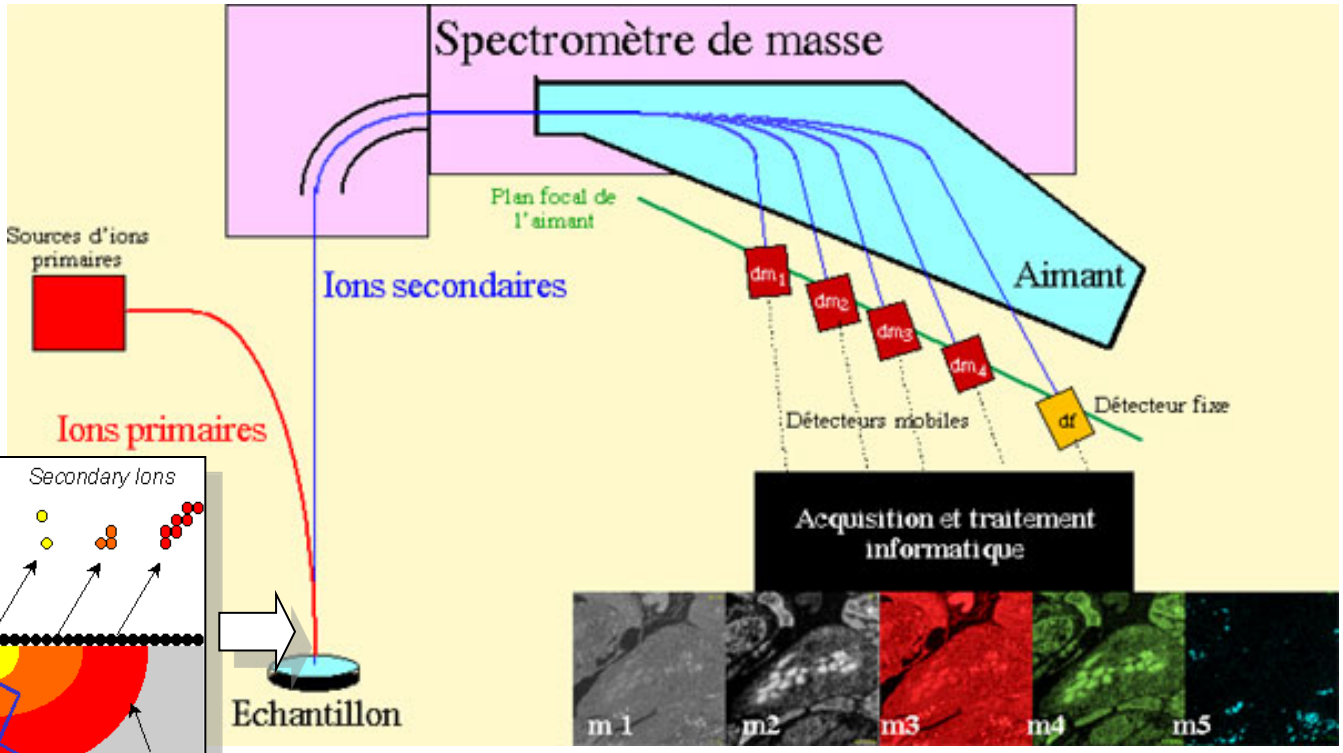
Computer assisted 3-D reconstruction of the corpus callosum



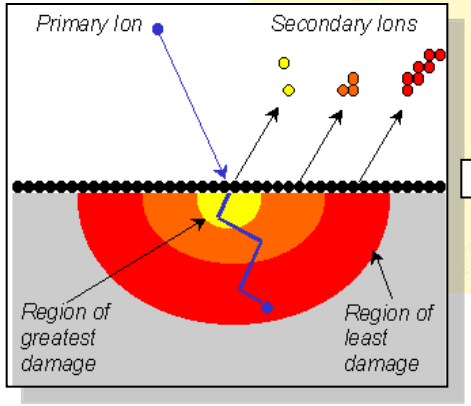


Bobby Bodenheimer, Department of Electrical Engineering and Computer Science at Vanderbilt University

Secondary ion mass spectrometer



Institut Curie, France



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Mass Spectrometry
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Imaging and differentiation of mouse embryo tissues by ToF-SIMS

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Received 1 June 2006; received in revised form 11 September 2006; accepted 11 September 2006

Abstract

Time-of-flight seconda
differentiate tissue types (
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principal component anal
embryos can be differenti
determine subtle chemica
Published by Elsevier B.V

Keywords: ToF-SIMS; Mou

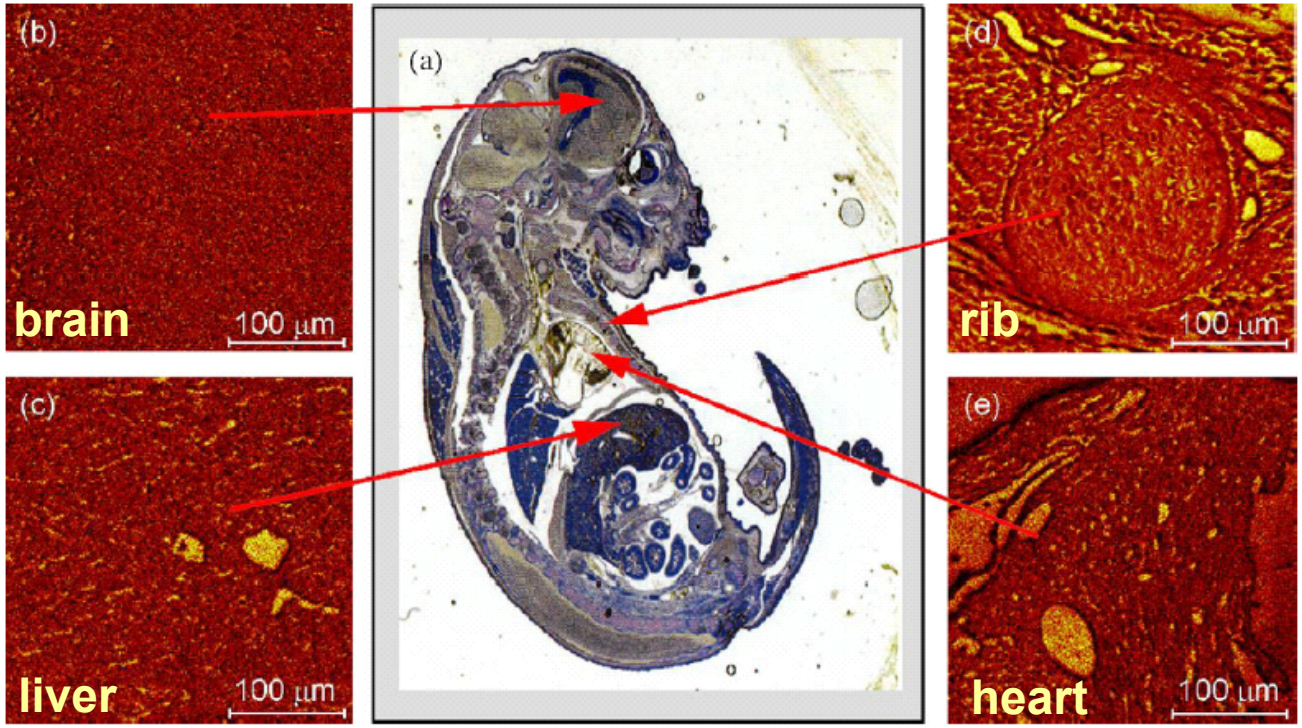


Fig. 1. (a) Optical image of a 16-day-old H&E stained mouse embryo section. (b) Positive total ion ToF-SIMS image of brain. (c) Positive total ion ToF-SIMS image of liver. (d) Positive total ion ToF-SIMS image of rib. (e) Positive total ion ToF-SIMS image of heart. Arrows point to the corresponding tissue region in the optical image.

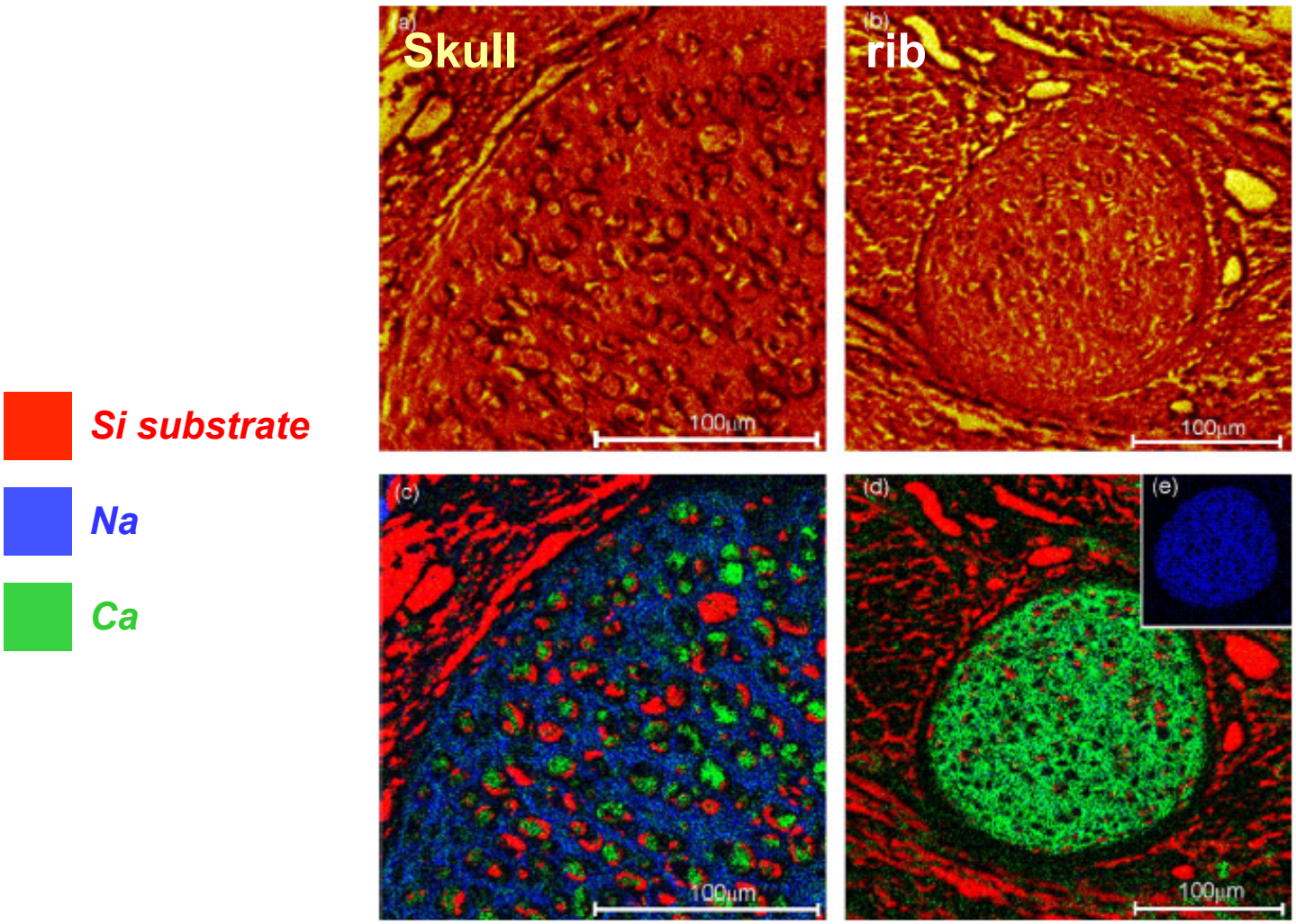
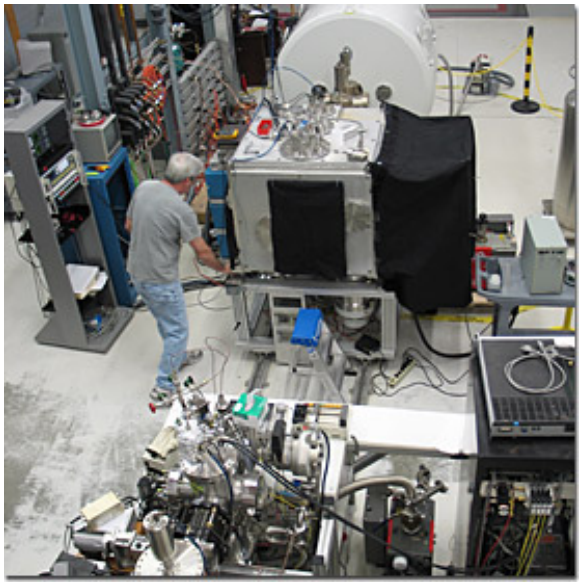


Fig. 5. (a) ToF-SIMS positive total ion image of a region of the skull. (b) ToF-SIMS positive total ion image of a rib. (c) Three-color overlay of the skull image; red color represents the Si substrate; green color represents the Na distribution; blue color represents the Ca distribution. Na and Ca are plotted on the same scale: (d) three-color overlay of the rib image, red color represents the Si substrate; green color represents the Na; blue color (too low to be visible) represents the Ca distribution. Na and Ca are plotted on the same scale: (e) Ca distribution with the signal intensity increased 5×.

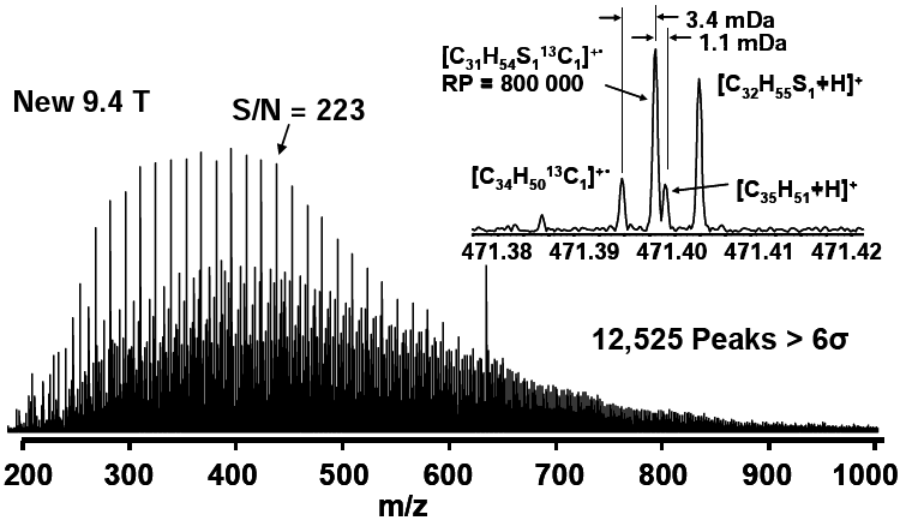
How to choose a suitable MS?

- Very low sample amount: go for MALDI.
- Require high mass accuracy: FTMS, TOF MS
- MS2 and high mass accuracy: TOF/TOF MS
- MS3 and above: ion trap (definitely FTICR if need high mass accuracy)

Petrochemical Application of FT-ICRMS



A. G. Marshall, National High Magnetic Field Lab,
Florida State University, USA.



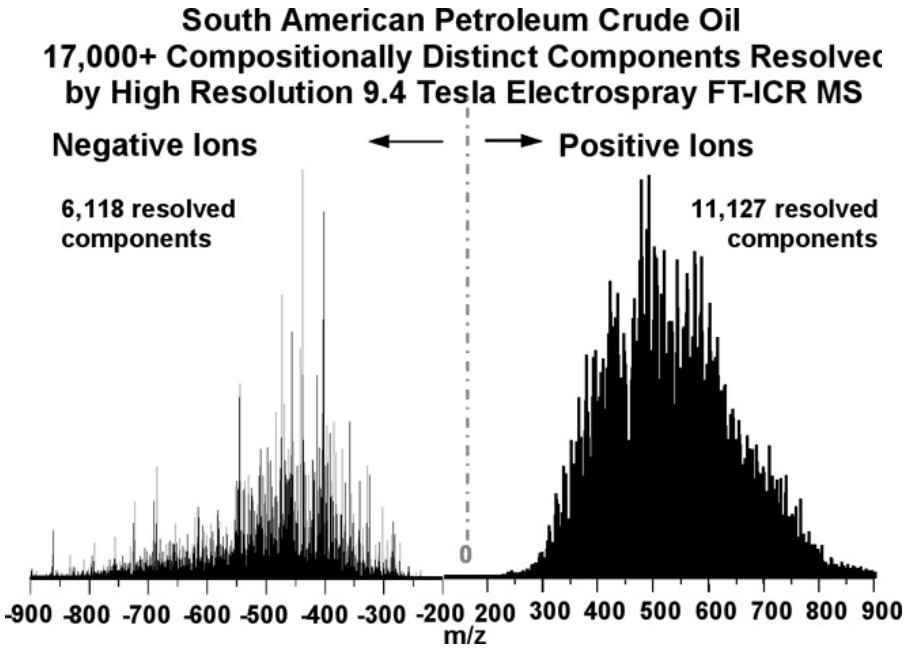


Figure 1. Positive-ion atmospheric pressure photoionization mass spectrum of a Middle Eastern light crude oil, acquired with the new NHMFL 9.4 T FT-ICR mass spectrometer. The inset illustrates resolution of the mass splits (1.1 mDa and 3.4 mDa) required for unequivocal identification of sulfur-containing components in petroloeum heavy crude oils.

Ultra High Resolution FT-ICRMS

Evgenij *Nikolaev*

J. Am. Soc. Mass Spectrom. (2011) 22:1125–1133
DOI: 10.1007/s13361-011-0125-9

RESEARCH ARTICLE

Initial Experimental Characterization of a New Ultra-High Resolution FTICR Cell with Dynamic Harmonization

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[1]The Institute for Energy Problems of Chemical Physics, Russian
Russia119334
[2]Institute of Biochemical Physics, Russian Academy of Sciences, M
[3]The Institute of Biomedical Chemistry, Russian Academy of Medi
[4]Bruker Daltonik GmbH, Bremen, Germany

Abstract

A new Fourier transform ion cyclotron resonance
principles of formation of the effective electric potentia
and Nikolaev (Proceedings of the 58th ASMS Confer
Commun Mass Spectrom 25:122–126, 2011) is co
operation is based on the concept of electric potent
cyclotron motion. Such an averaging process permits
entire volume of a cylindrical Penning trap to be equa
hyperbolic electrodes in an ideal Penning trap. The
new cell are shaped for generating a quadratic depend
(along cyclotron motion orbit) electric potential at ar
electrodes together with the trapping segments form
cylindrical cell. In excitation mode this cell being
cylindrical cell of the same length. It is more effecti
cyclotron radii than a Gabrielse et al.-type (Int J Ma
1989) cylindrical cell with four compensation section
twenty millions of reserpine (*m/z* 609) and more t
molecular ions (*m/z* 1357) has been obtained in a 7T

Key words: FT ICR MS, Penning trap, Dynamic harm

Resolving Power: > 10^7

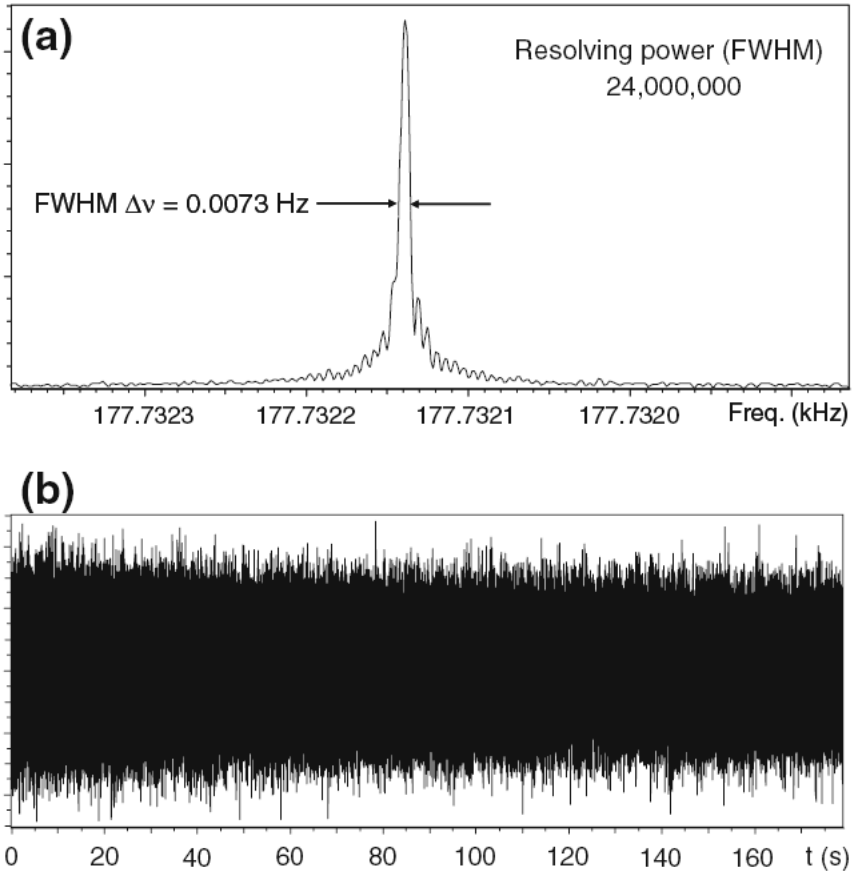

Figure 2. (**a**) Frequency spectrum (not calibrated) of the mono isotopic peak of singly charged, protonated reserpine (*m/z* 609.28066) with a resolving power of 24,000,000, resulting from magnitude FFT calculation without apodization. (**b**) Time domain spectrum of reserpine, detected over 3 min

Important Topics of MS Development

- New ionization method for carbohydrates;
- New fragmentation methods, i.e. site-specific cleavage for oligosaccharides.
- Reliable method for quantitative measurements;
- Ion detector for high mass molecules;
- Miniaturization;

Useful References

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Edmond de Hoffmann, Vincent Stroobant, JohnWiley & Sons, LTD., Chichester, 2001.

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