

Mass spec & Proteomics

Do elephants fly ?



Ciências
ULisboa

Ionização

- MALDI

Matrix Assisted Laser Desorption Ionization

- ESI

ElectroSpray Ionization



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graph LR; Fonte --> Selector; Selector --> Detector;
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Fonte → Selector → Detector

MALDI



Koichi Tanaka
*2002 Nobel Prize for
Chemistry
(Development of
MALDI ionisation for
biological analysis)*

THE ORIGIN OF MACROMOLECULE IONIZATION BY LASER IRRADIATION

Nobel Lecture, December 8, 2002

by

KOICHI TANAKA

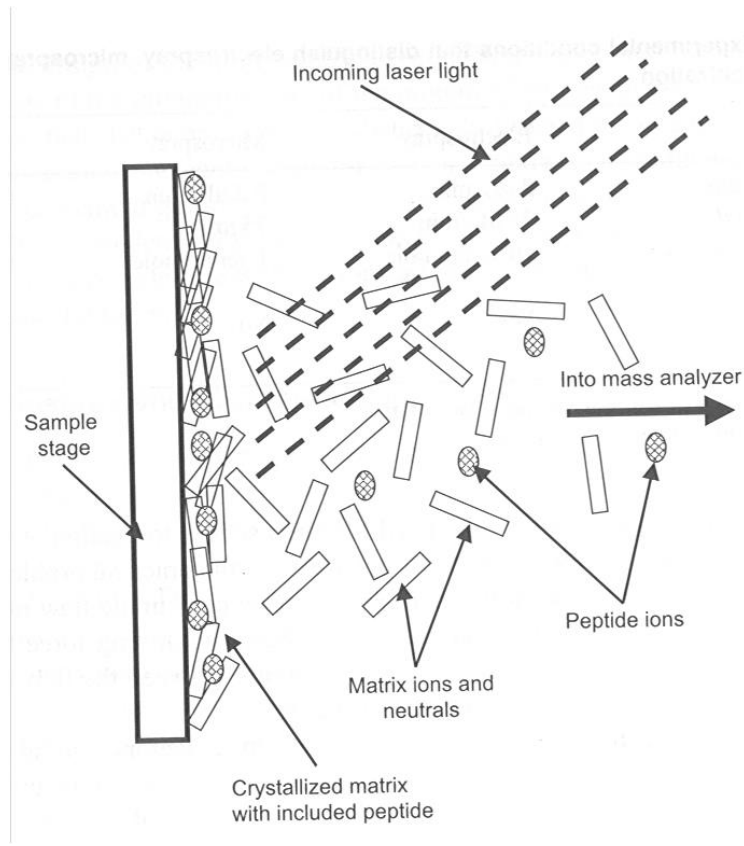
Shimadzu Corporation, 1 Nishinokyo-Kuwabaracho, Nakagyo-ku, Kyoto 604-8511, Japan.

INTRODUCTION

When I was a student at university, my major field of study was Electrical Engineering. I did not specialize in chemistry in my studies at university, and my knowledge of chemistry overall was somewhat less than rich. Under those circumstances, upon entering the company, I applied myself wholeheartedly to the study of chemistry to challenge and overcome a barrier in analytical chemistry considered to be impenetrable. I am, of course, very pleased to re-

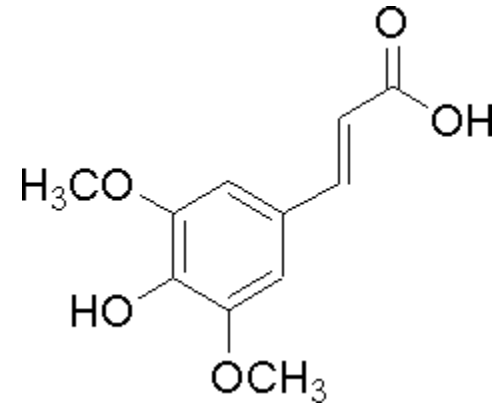
MALDI

**Matrix
Assisted
Laser
Desorption
Ionization**

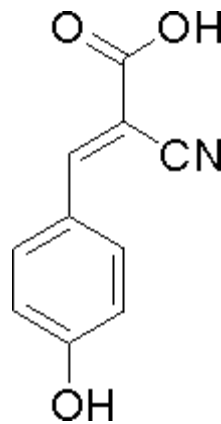


PROTEÍNAS

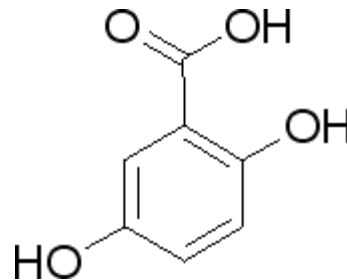
Ácido sinapínico
(SA)



Ácido α -ciano-4-hidroxicinámico
(HCAC)

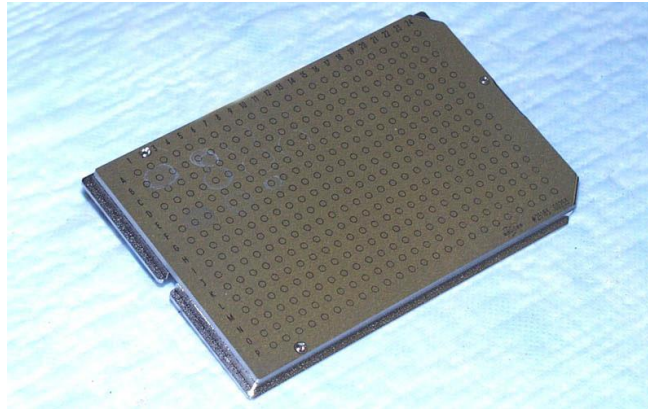


Ácido 2,5-Dihidroxibenzóico
(DHB)

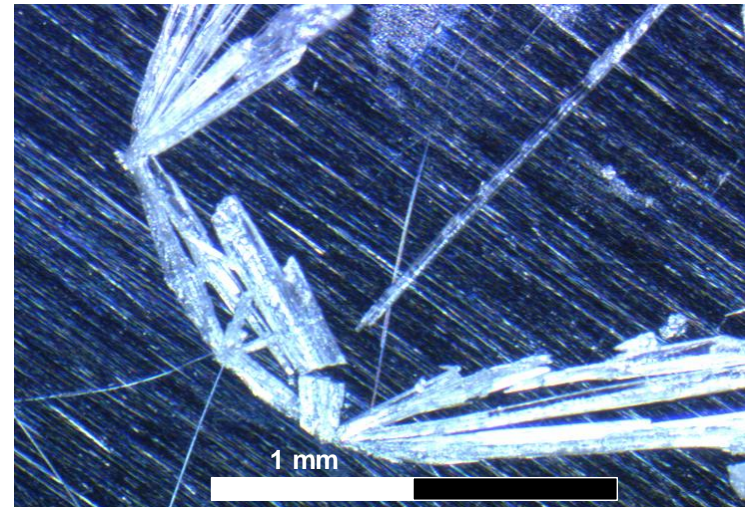
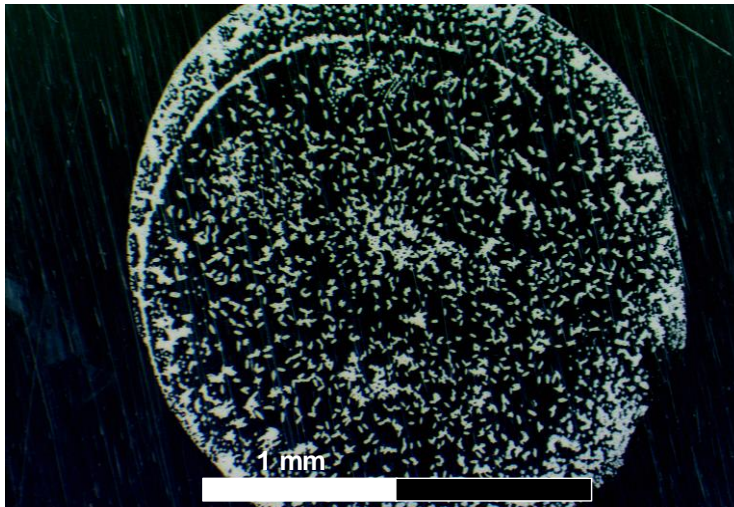


PÉPTIDOS

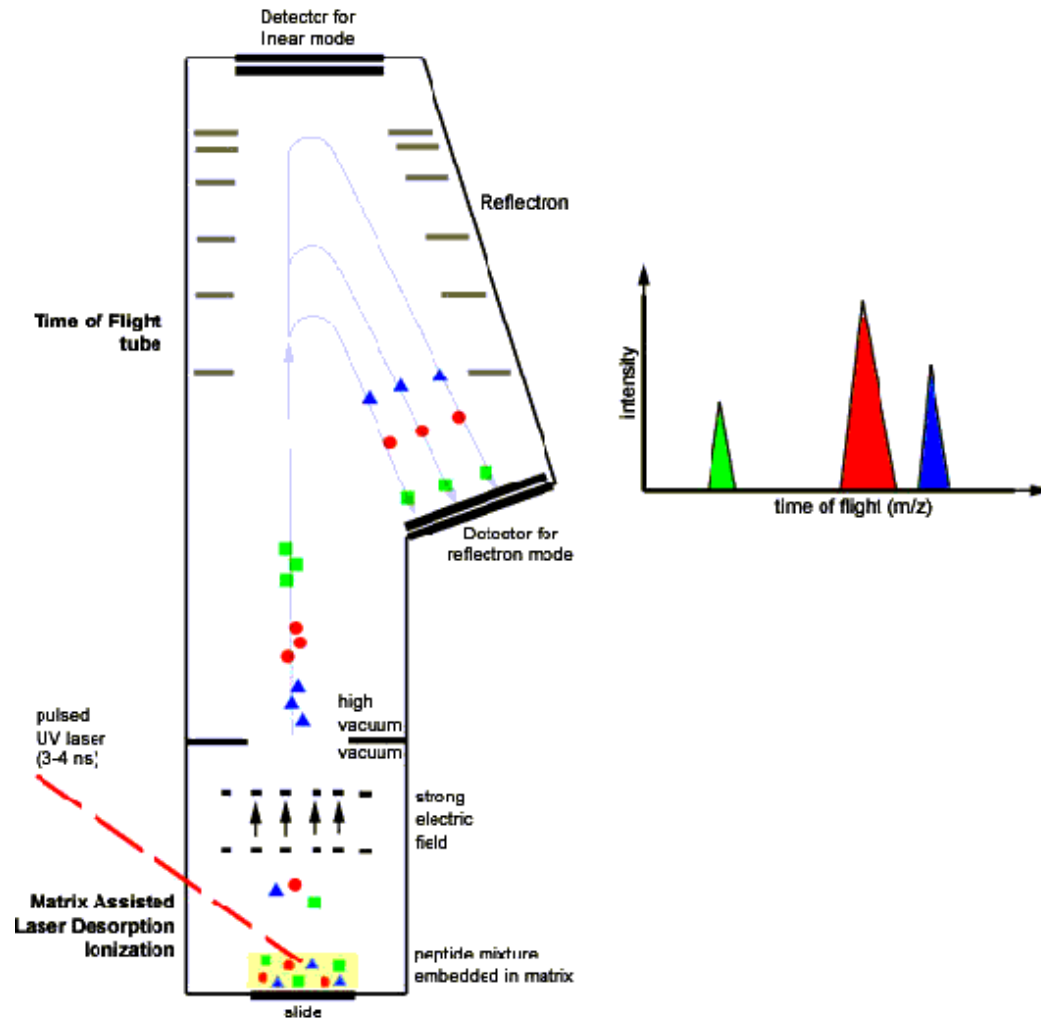
MALDI
Target



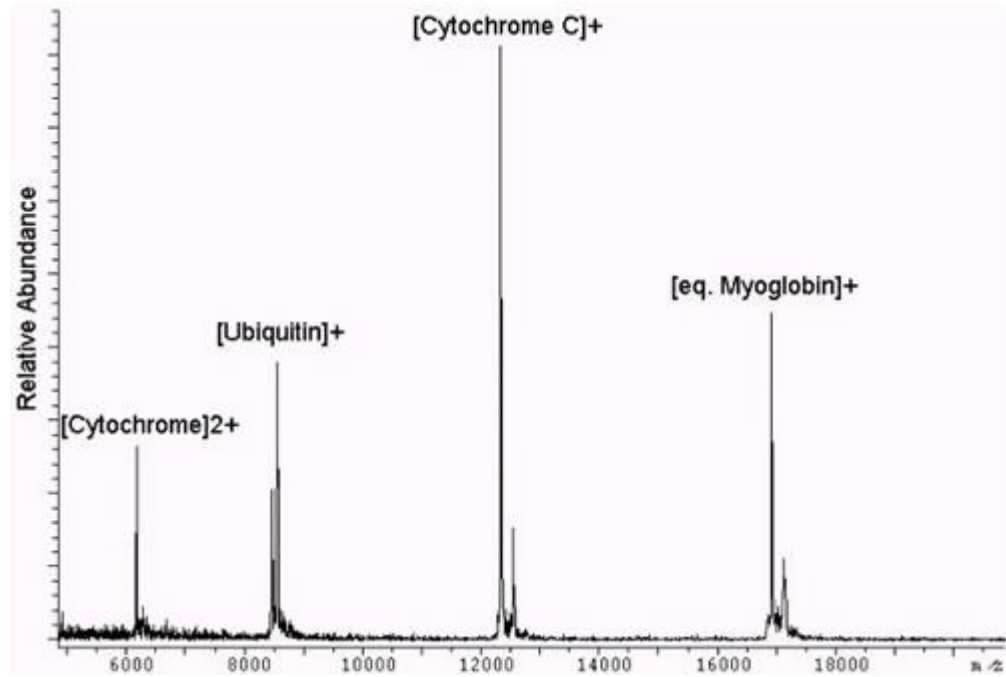
MALDI
spot



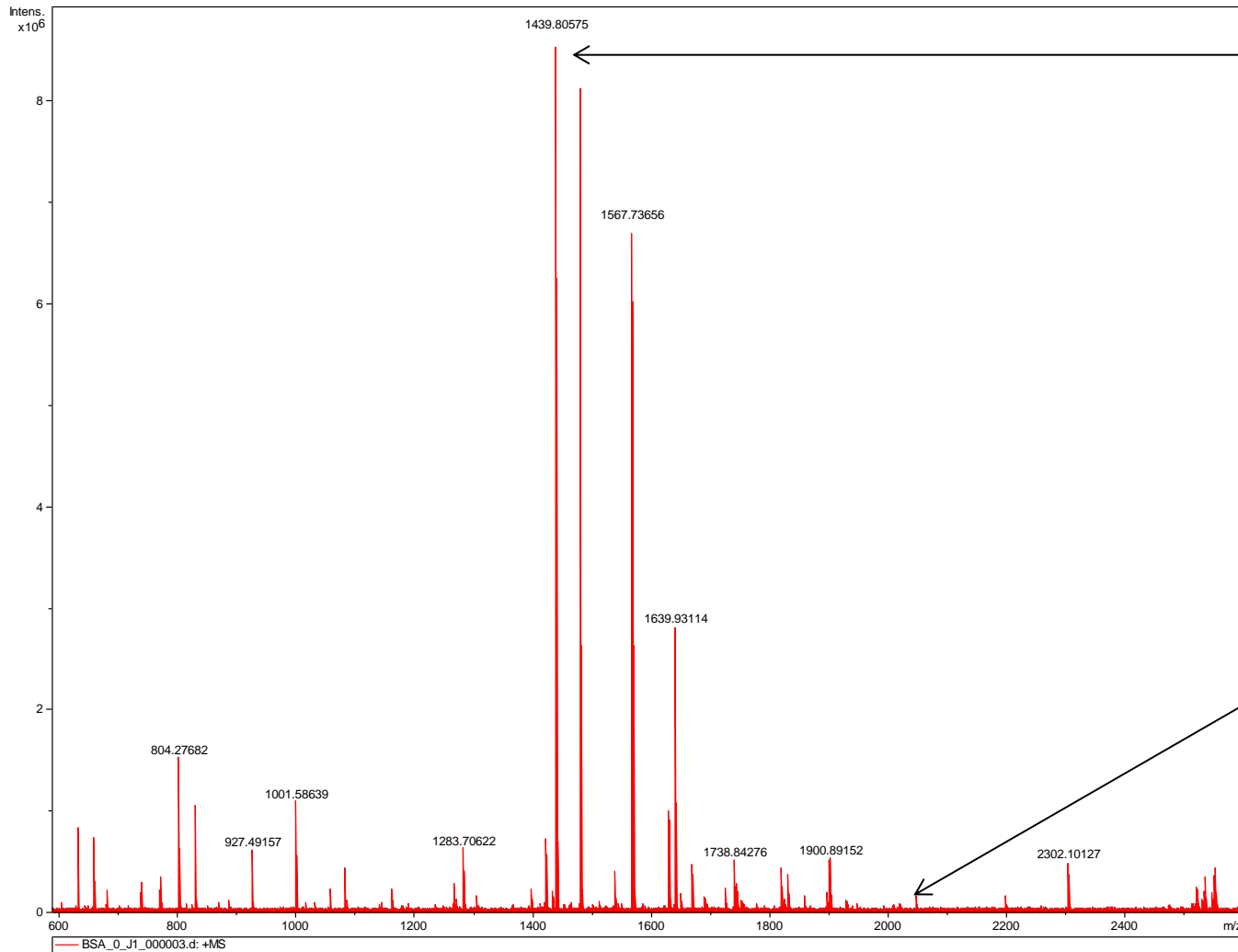
TOF – Time of Flight



Protein mix



Peptide mapping



RHPEYAVSVLLR

RHPYFYAPELLYYANK

MALDI

- Ionização robusta
- Espectros simples (1 carga)
- Limite de detecção (amol)
- $m/z > 1000$

ESI



John Bennet Fenn
*2002 Nobel Prize for
Chemistry
(Development of ESI
ionisation for
biological analysis)*

ELECTROSPRAY WINGS FOR MOLECULAR ELEPHANTS

Nobel Lecture, December 8, 2002

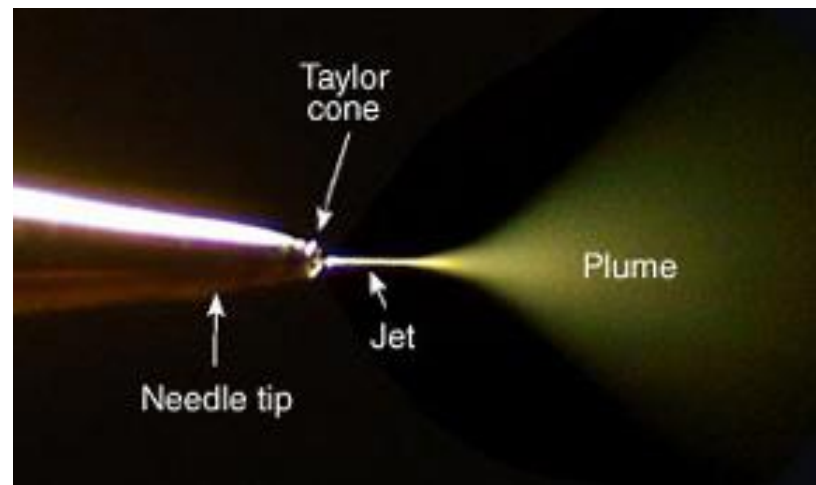
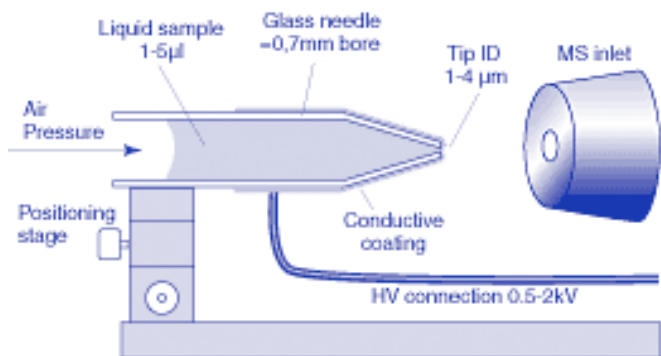
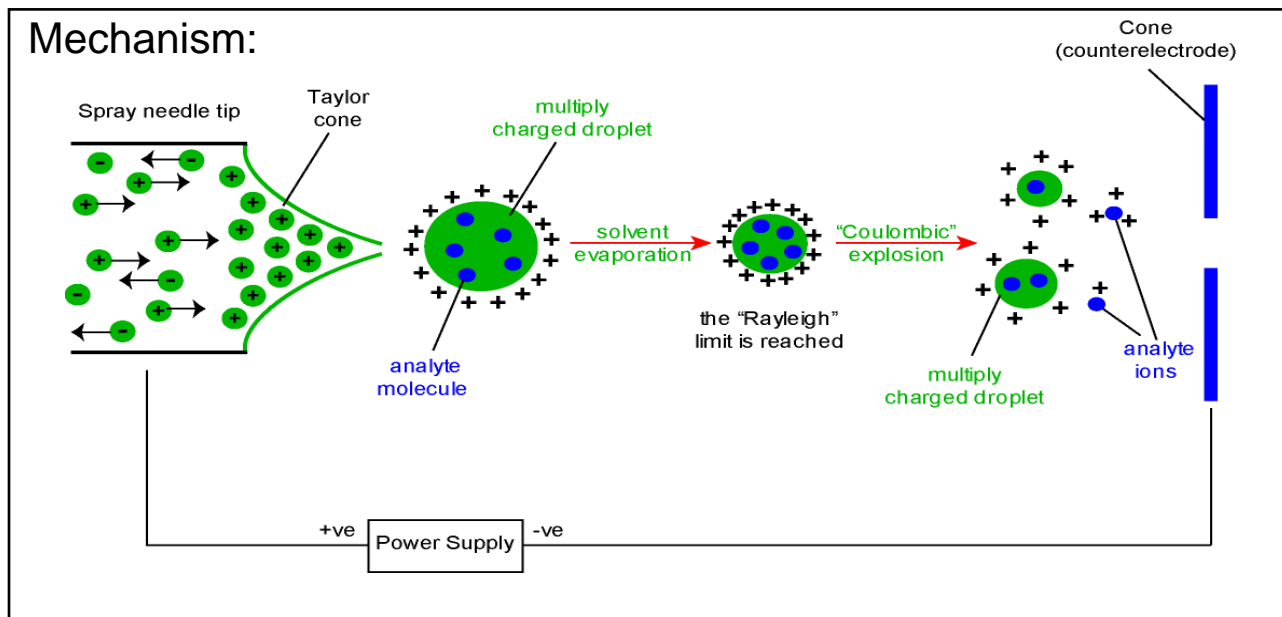
by

JOHN B. FENN

Department of Chemistry, Virginia Commonwealth University, Richmond,
Virginia 2384-2006, USA.

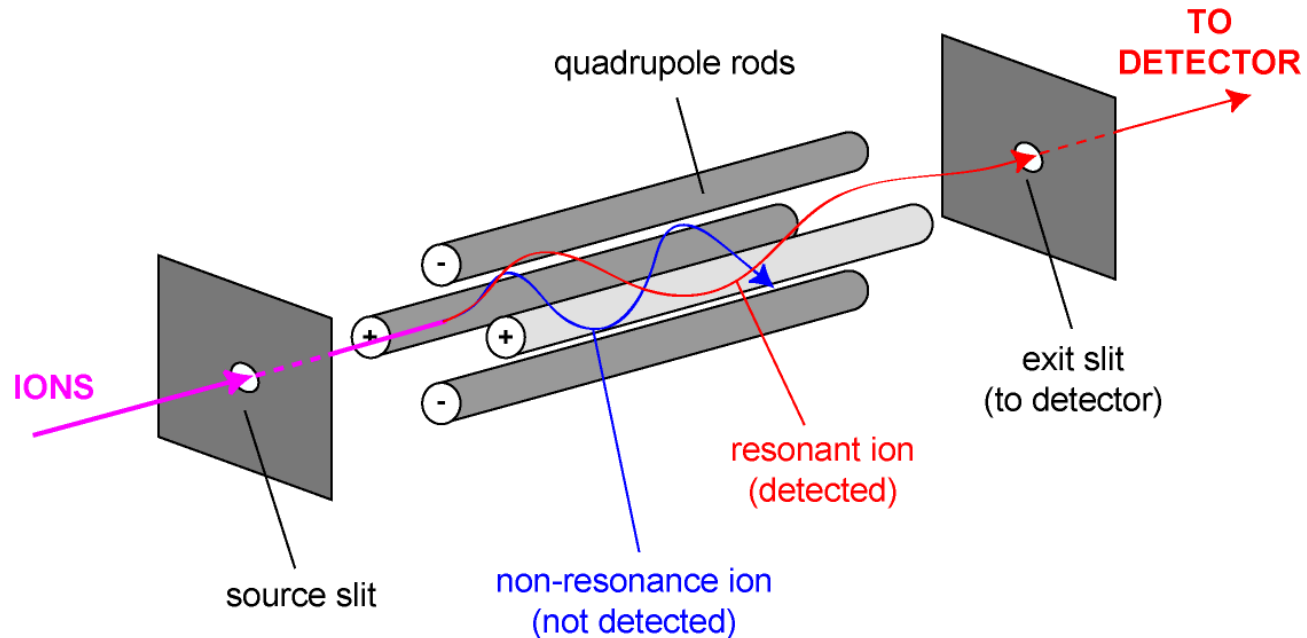
The grant from NSF in 1960 started us on the road that led to Stockholm in 2002. Co-Principal Investigator, Michel Boudart was then hosting Jacques

Electro Spray Ionisation



Analísadores de Massa

■ Quadrupolo



Analísadores de Massa

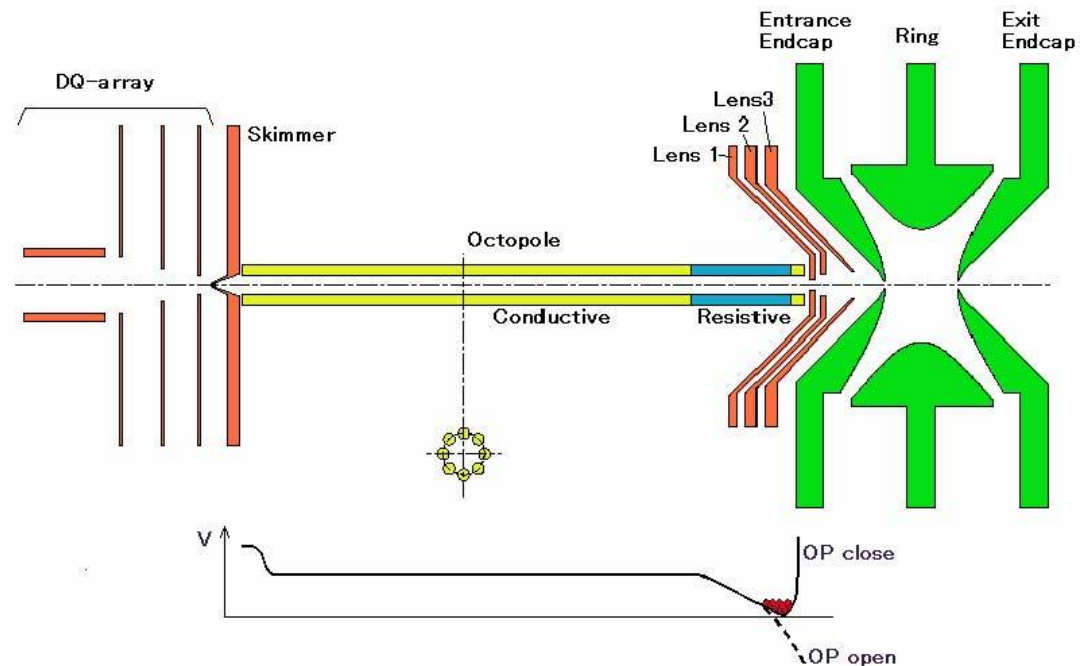
■ *Paul's trap*



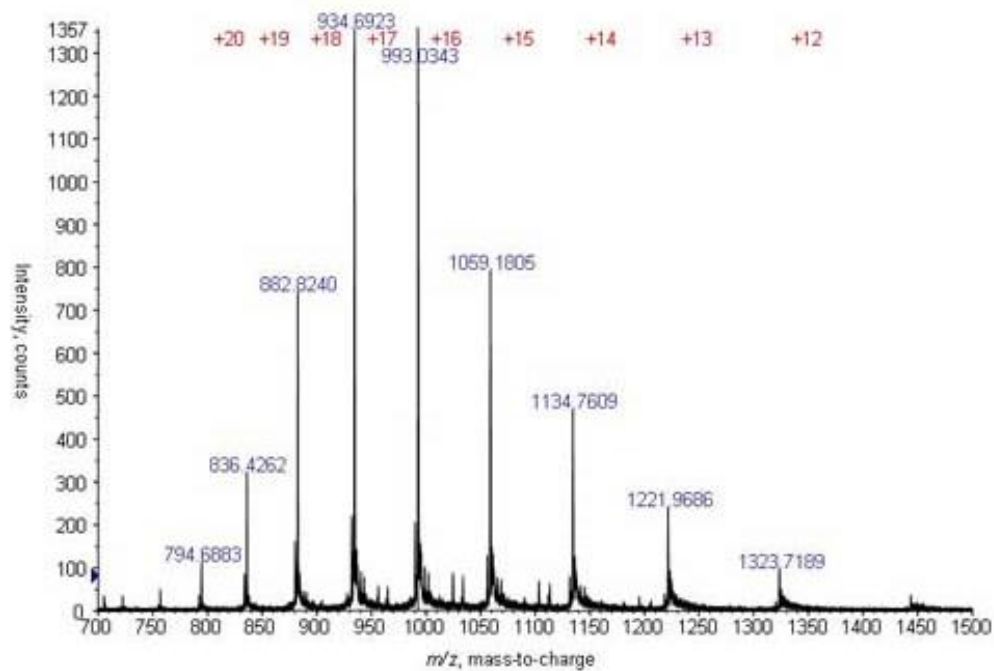
W. Paul

1989 Nobel Prize for
Physics

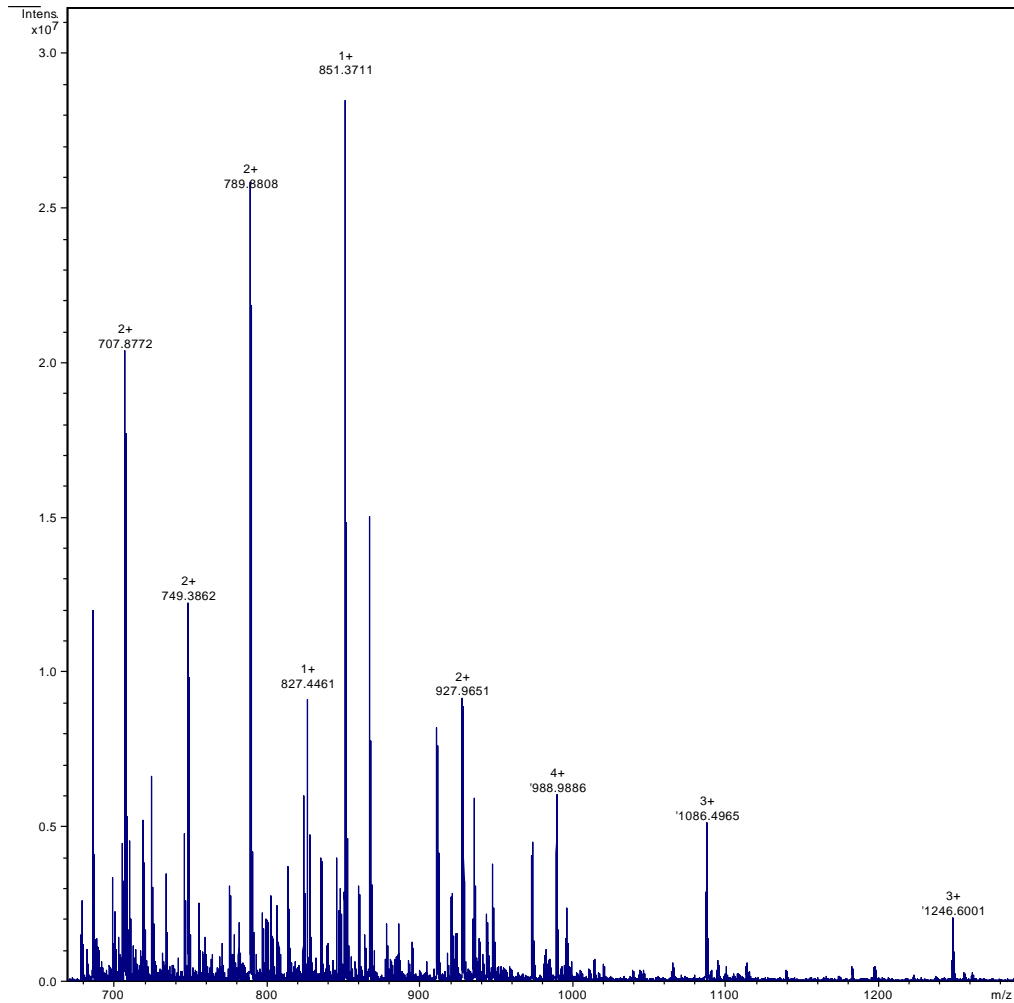
(Development of the
ion trap)



ESI – Proteína (15 kDa)



ESI – Peptide mapping





Algoritmos e software...

- Charge deconvolution
 - Maximum entropy methods

- Average / Monoisotopic
 - m/z
 - SNAP

ESI

- Ionização sensível a contaminantes
- Espectros muito complexos ($m/z > 1$)
- Mantém interações não covalentes
- Supressão de sinal
- Optimização de condições
 - pH
 - Solvente
 - Concentração



Conceitos

Fundamentais!

Exactidão de massa

$$\frac{\Delta m}{m} \cdot 10^6 \quad (\text{ppm})$$

100,0

100,00

100.0000

100.1

100.01

100.0001

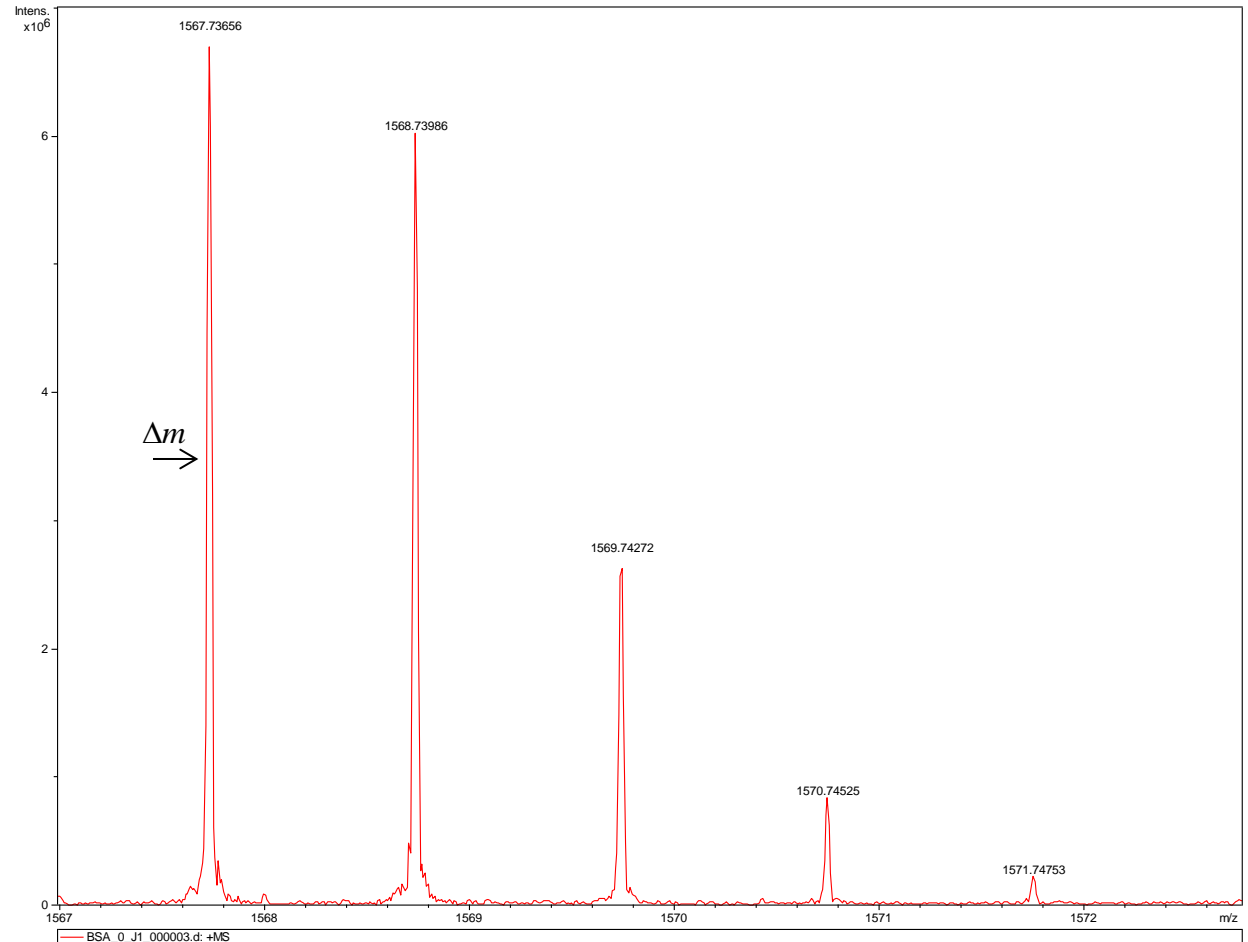
1000 ppm

100 ppm

1 ppm

Resolução

$$R = \frac{m}{\Delta m}$$



Resolving power

