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Ion Mobility Spectrometry (IMS): Instrumentation and Application

by

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Isfahan Scientific and Research Town

Mohammad Taghi Jafari

Date of Birth: March, 22, 1976

Marital Status: Married and blessed by one daughter (Elena)

- Professor – from Winter 2019 (IUT)
- Associate Professor – from Spring 2012 (IUT)
- Head of Central Laboratory -- Summer 2008-summer 2018 (IUT)
- Assistant Professor – from Summer 2007 (IUT)

College of Chemistry, Isfahan University of Technology,
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Teif Azmon Espadana Co.
E-mail: teifazmon@gmail.com URL: www.teifazmon.com

Education

2002-06 Ph.D.: Analytical Chemistry

Field: Analytical Instrumentation

Title: ***Design and construction of electrospray ionization - ion mobility spectrometry (ESI-IMS) and analysis of antibiotics, furfurals and … using ion mobility spectrometry with corona discharge as the ionization source.***

Department of Chemistry, Isfahan University of Technology, Isfahan, I.R. Iran

1999-02 M.Sc.: Analytical Chemistry

Field: Chemical Analysis

Title: ***Analysis of explosives by ion mobility spectrometry using corona discharge as ionization source.***

Department of Chemistry, Isfahan University of Technology, Isfahan, I.R. Iran

1994-98 B. Sc.: Chemistry

Field: Applied Chemistry

Department of Chemistry, Isfahan University, Isfahan, I.R. Iran

Publications and Students

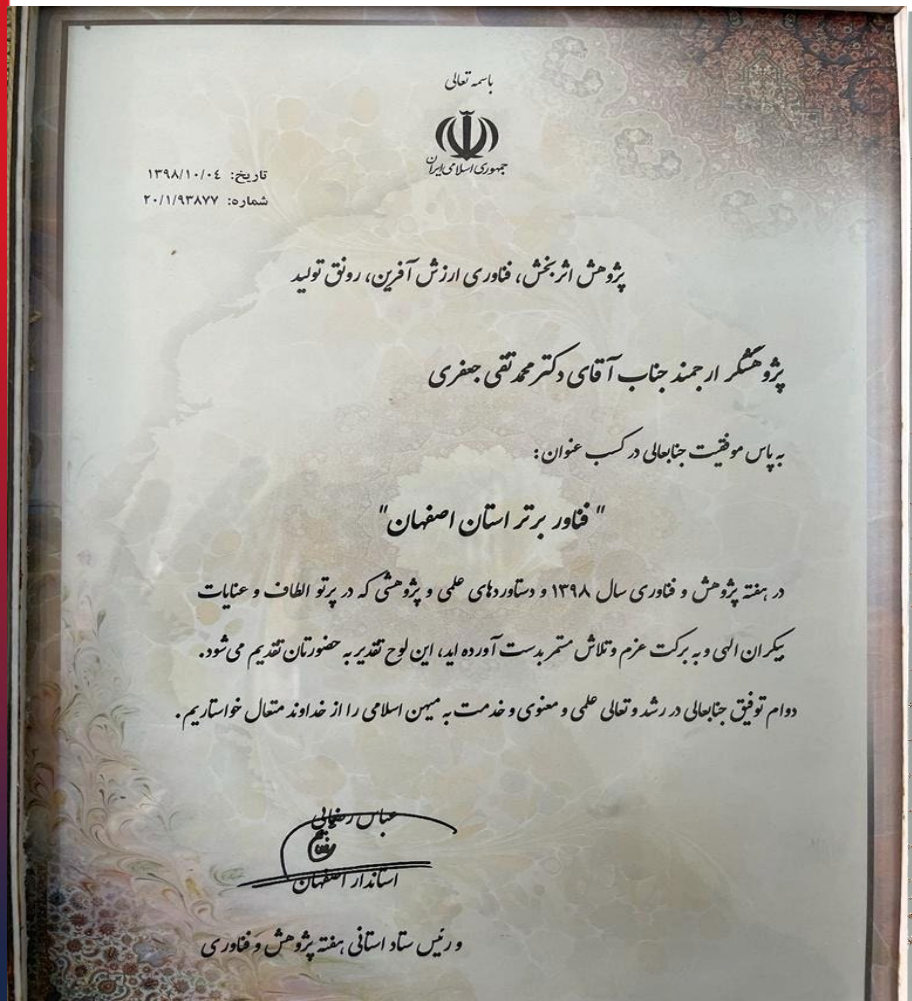
MSc Students: 50
PhD Students: 12

~ 70 ISI paper:
Anal. Chem.
Anal. Chim. Acta
J. Chromatog. A
Talanta
Food Chem.

14 Patent, all related to IMS

New Honors & Awards

The Distinguished Technologist of the year award in *Isfahan Province*, (Isfahan, Iran), Dec., 2019.



باسمه تعالی

جمهوری اسلامی ایران

تاریخ: ۱۳۹۸/۱۰/۰۴
شماره: ۲۰/۱/۹۳۸۷۷

پژوهش اثربخش، فناوری ارزش آفرین، رونق تولید

پژوهشگر ارجمند جناب آقای دکتر محمد تقی جعفری

به پاس موفقیت جنابعالی در کسب عنوان:

"فناور برتر استان اصفهان"

در هفته پژوهش و فناوری سال ۱۳۹۸ و دستاوردهای علمی و پژوهشی که در پرتو الطاف و عنایات یکتای الهی و به برکت عزم و تلاش مستمر بدست آورده اید، این لوح تقدیر به حضورتان تقدیم می شود.

دوام توفیق جنابعالی در رشد و تعالی علمی و معنوی و خدمت به میهن اسلامی را از خداوند متعال خواستاریم.

عباس رضایی
استاندار اصفهان

و رئیس ستاد استانی هفته پژوهش و فناوری

Third position in the ranking of startups, Isfahan Science and Technology, 2017.

شرکت علمی و تحقیقاتی اصفهان

لوح تقدیر

جناب آقای دکتر محمد تقی جعفری

مدیر عامل محترم شرکت طیف آزمون اسپادانا

تلاش مستمر جنابعالی و همکارانتان در راستای رشد و تعالی اقتصاد و فناوری ایران عزیز، از طریق ایجاد و توسعه کمی و کیفی آن شرکت فناور ستودنی است. اکنون که در ارزیابی دوره ای سال ۱۳۹۶ در گروه واحدهای فناوری کمتر از یک سال استقرار در مراکز رشد شرکت علمی و تحقیقاتی اصفهان موفق به کسب رتبه سوم شده اید، دستیابی به این توفیق را صمیمانه تبریک گفته و تداوم آن را در راه بالندگی کشور از درگاه ایزد منان مسئلت دارم.

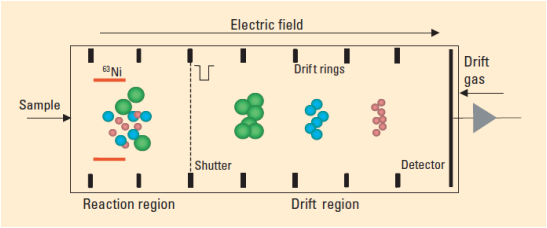
مهدی کشمیری
رئیس شرکت علمی و تحقیقاتی اصفهان
اردیبهشت ۱۳۹۷

Outline

- Introduction
  - ✓ Ion Mobility Spectrometry (IMS)
- Part A : Instrumentation
  - ✓Ionization Sources
    - ~ Corona Discharge (CD)
    - ~ Electrospray Ionization (ESI)
    - ~ Low Temperature Plasma (LTP)
  - ✓Drift Tube Design
  - ✓GC-IMS
- Part B : Application

Introduction

Ion mobility spectrometry (IMS) was introduced commercially as plasma chromatography in 1970.



Anal. Chem. 2004, 391A.

IMS is an accepted analytical method for qualitative and quantitative analysis of trace substances such as explosives, chemical weapons, and illicit drugs.

Portability, speed, low cost, ease of maintenance, and low detection limits (~ppb) are luring scientists to IMS.

www.monstermarketplace.com/air-monitor-equipment

www.laboratoryequipment.com

History

Drift Cell was first developed primarily by Earl W. McDaniel of Georgia Institute of Technology in the 1950s and 1960s.

IMS was applied by F. W. Karasek for chemical analysis in the 1970s.

Prof. Gary A. Eiceman

Prof. Herbert H. Hill

IMS Application

Various application fields:

- Military (> 50,000 used by US Army)

Anal. Chem. 2004, 391A.

- Environmental

www.elmulab.co.za

- Airport (> 10,000)

http://global-security-solutions.com/IonScanSentinel.html

- Space Shuttle

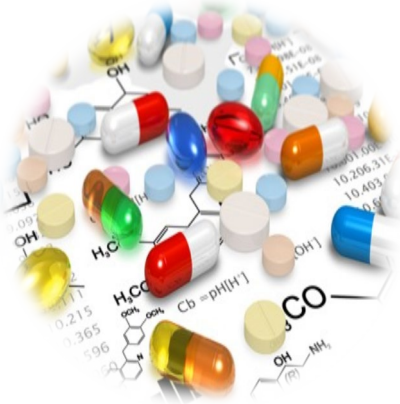
Anal. Chem. 2004, 391A.

Other Application

Pesticides
Insecticides
Herbicides

Environment

Essence

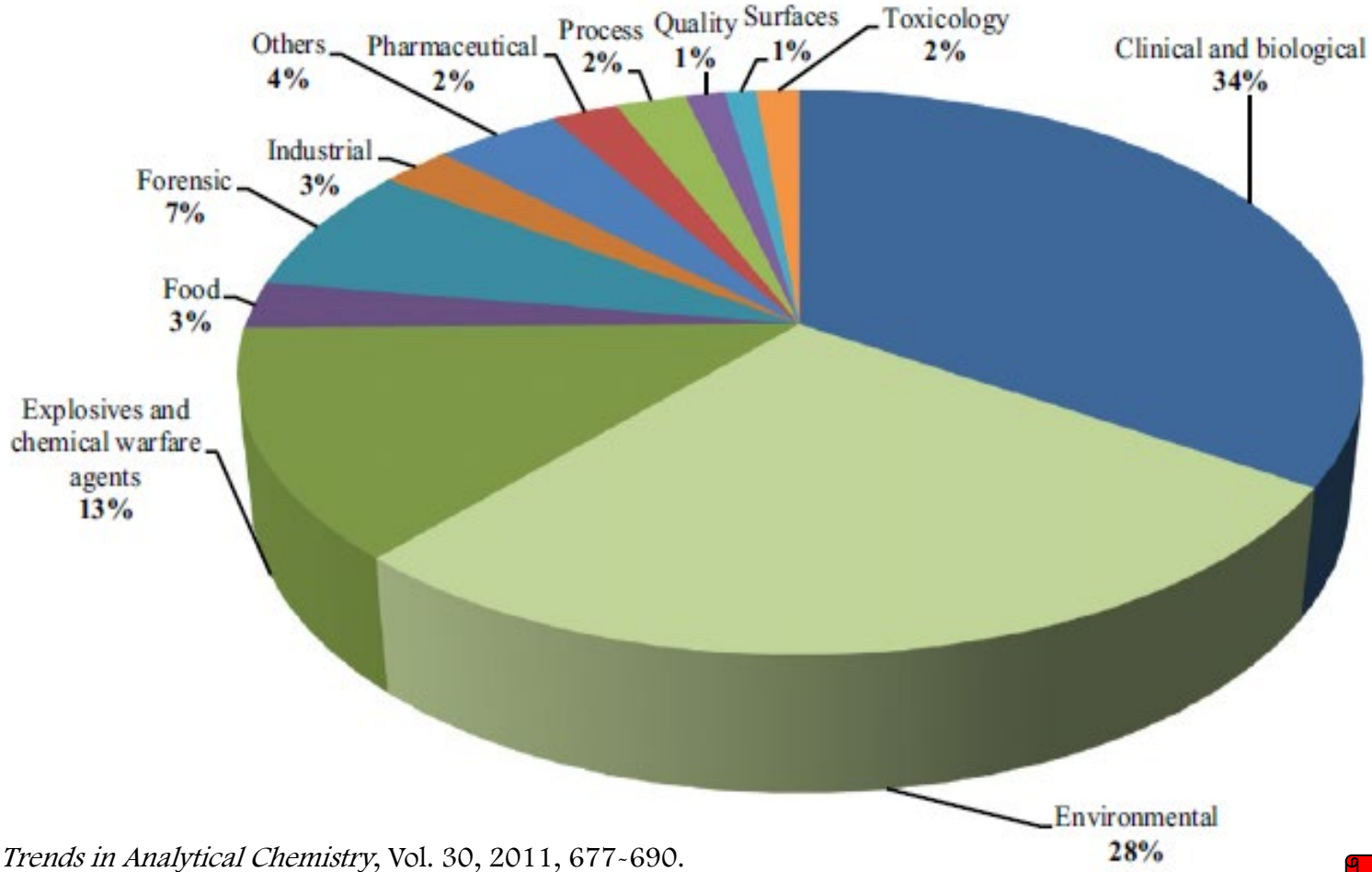


Clinical Drugs
Abuse Drugs

Fruits
Vegetable

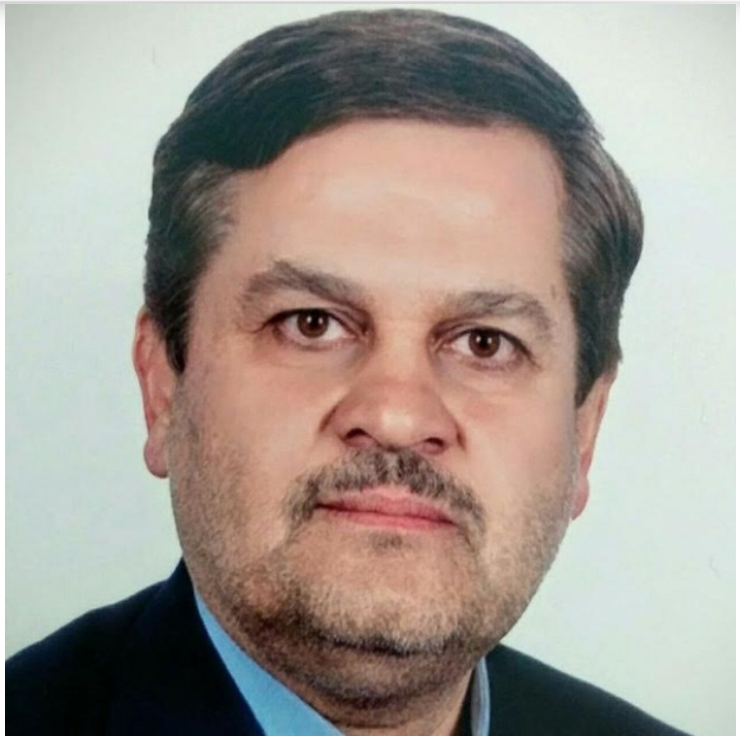
IMS Application

Contribution to different areas of study.
The percentages were calculated over 721 references (ISI Web of Knowledge, May 2010)



Trends in Analytical Chemistry, Vol. 30, 2011, 677-690.

IMS in Iran



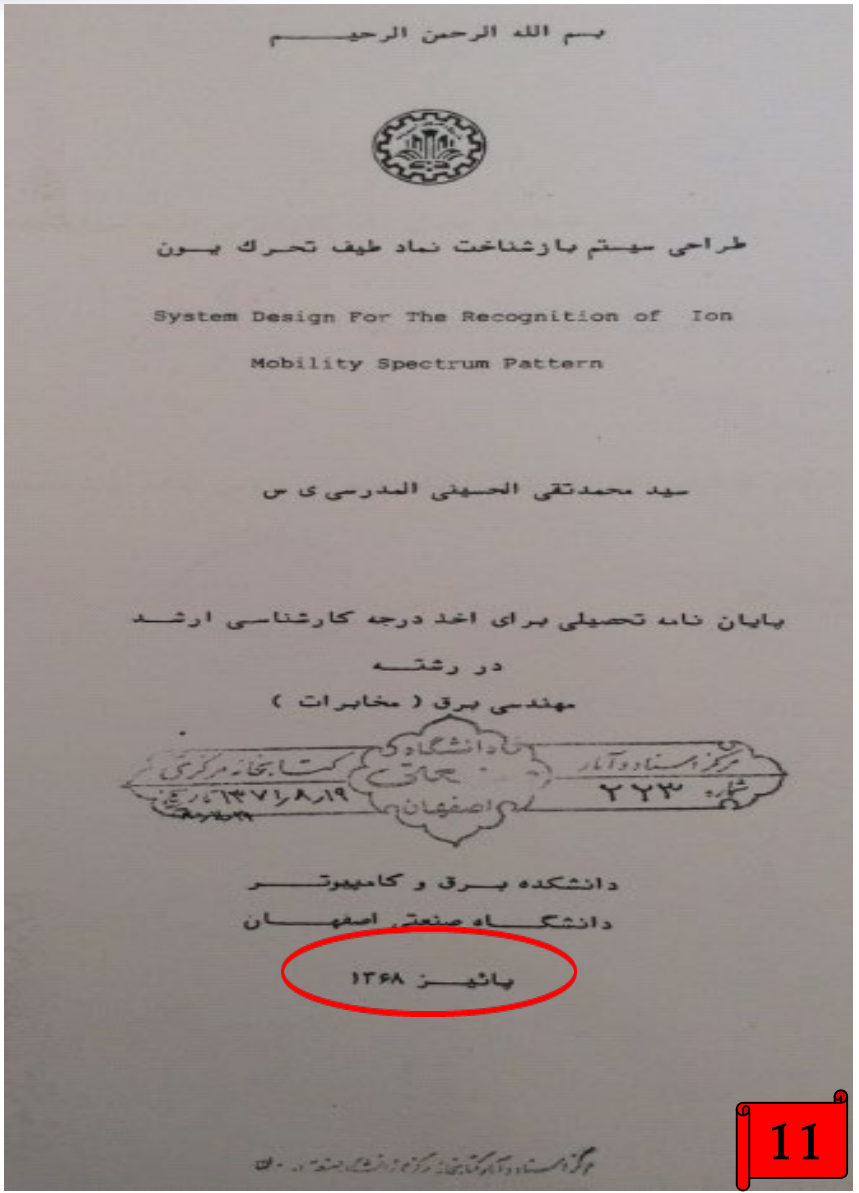
Dr. Almodarresi

Prof. A. DoostHoseini

Prof. T. Khayamian

Prof. M. K. Amini

Prof. M. Tabrizchi



بسم الله الرحمن الرحیم

طراحی سیستم بازشناخت نماد طیف تحرک یون

System Design For The Recognition of Ion Mobility Spectrum Pattern

سید محمدتقی الحسینی المدرسی ی س

پایان نامه تحصیلی برای اخذ درجه کارشناسی ارشد

در رشته

مهندسی برق (مخابرات)

دانشکده برق و کامپیوتر

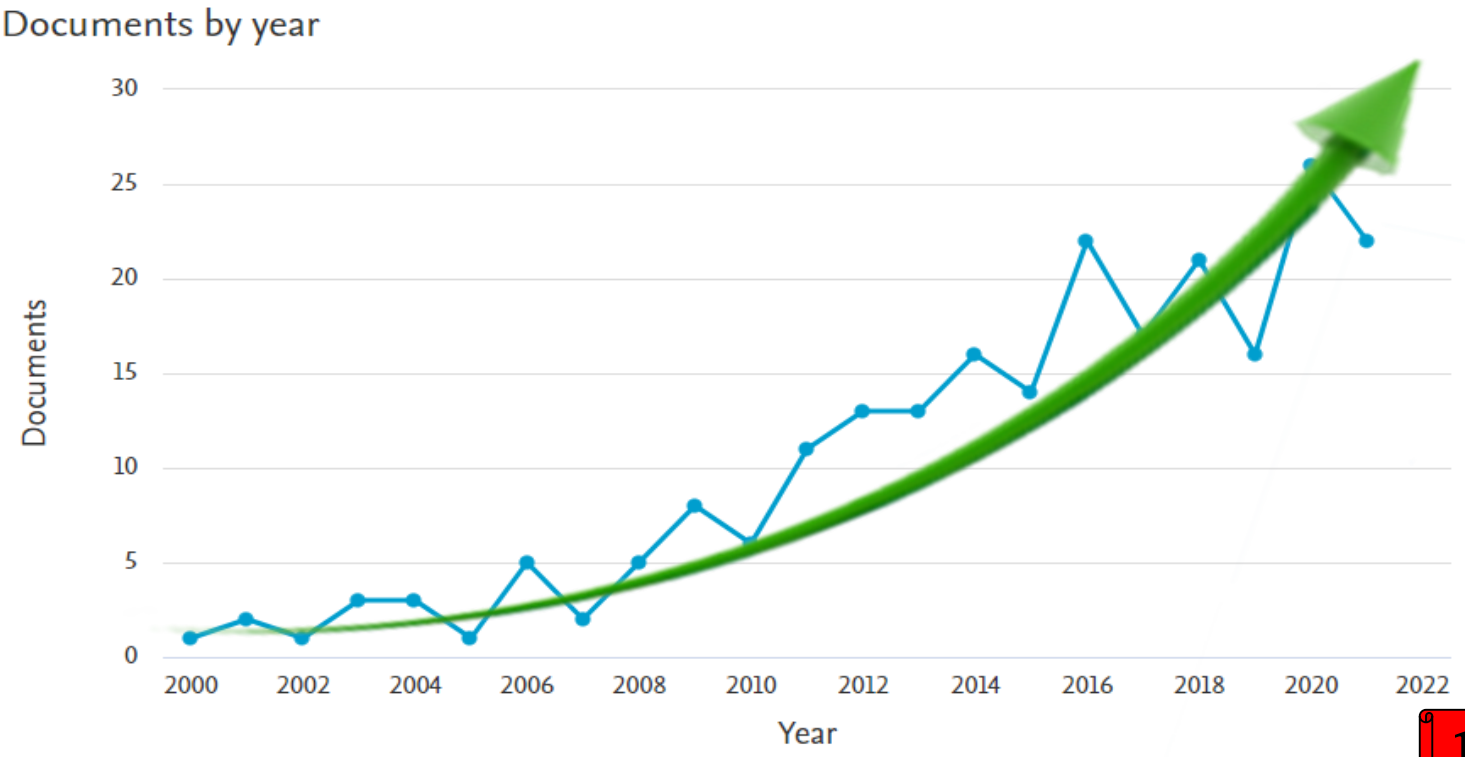
دانشگاه صنعتی اصفهان

پائیز ۱۳۶۸

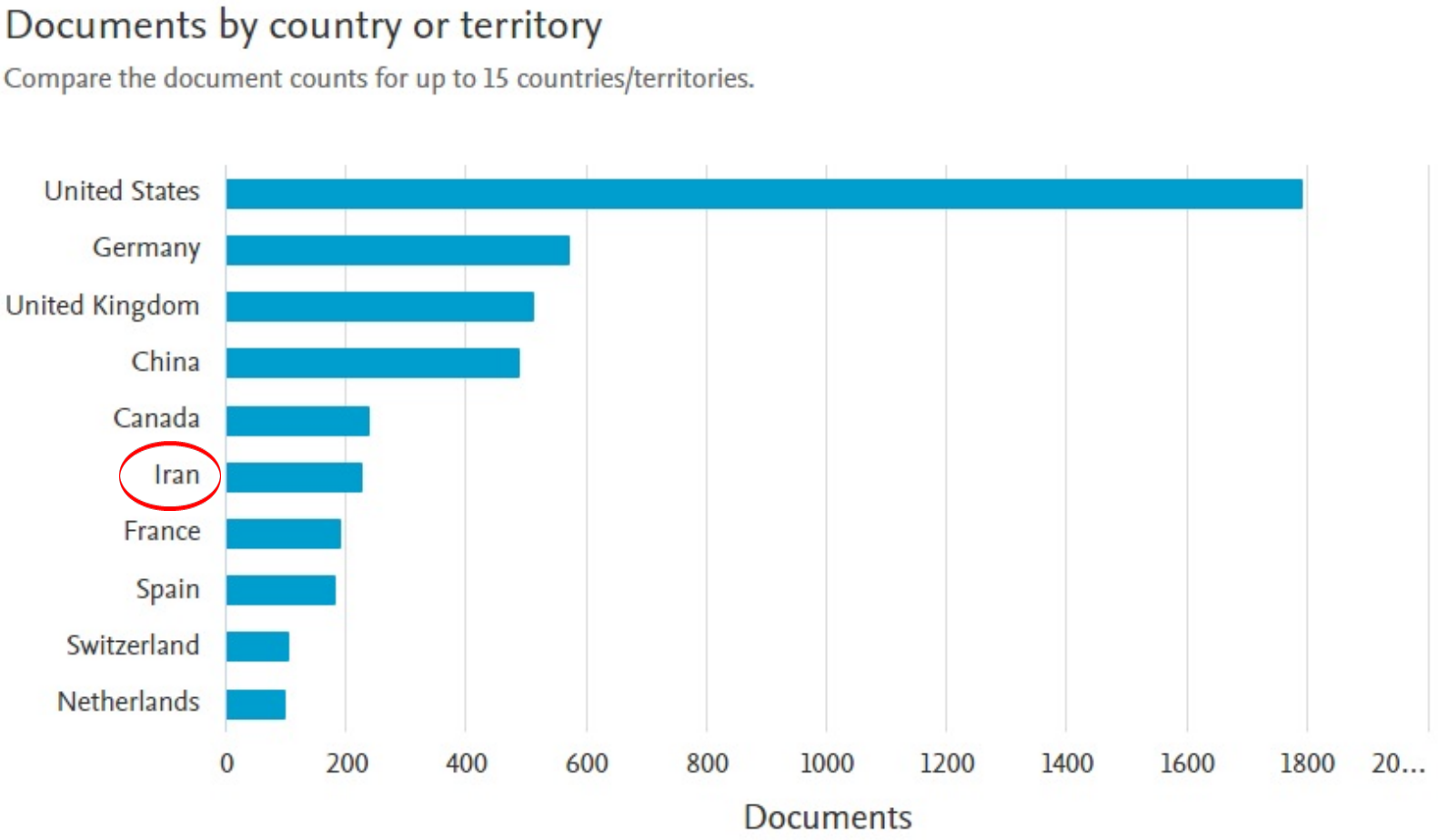
Publication

Over 4548 papers (60 Review articles), and 4 books.

Contribution of Iran is 228 papers.
(Scopus, 11 September, 2021)



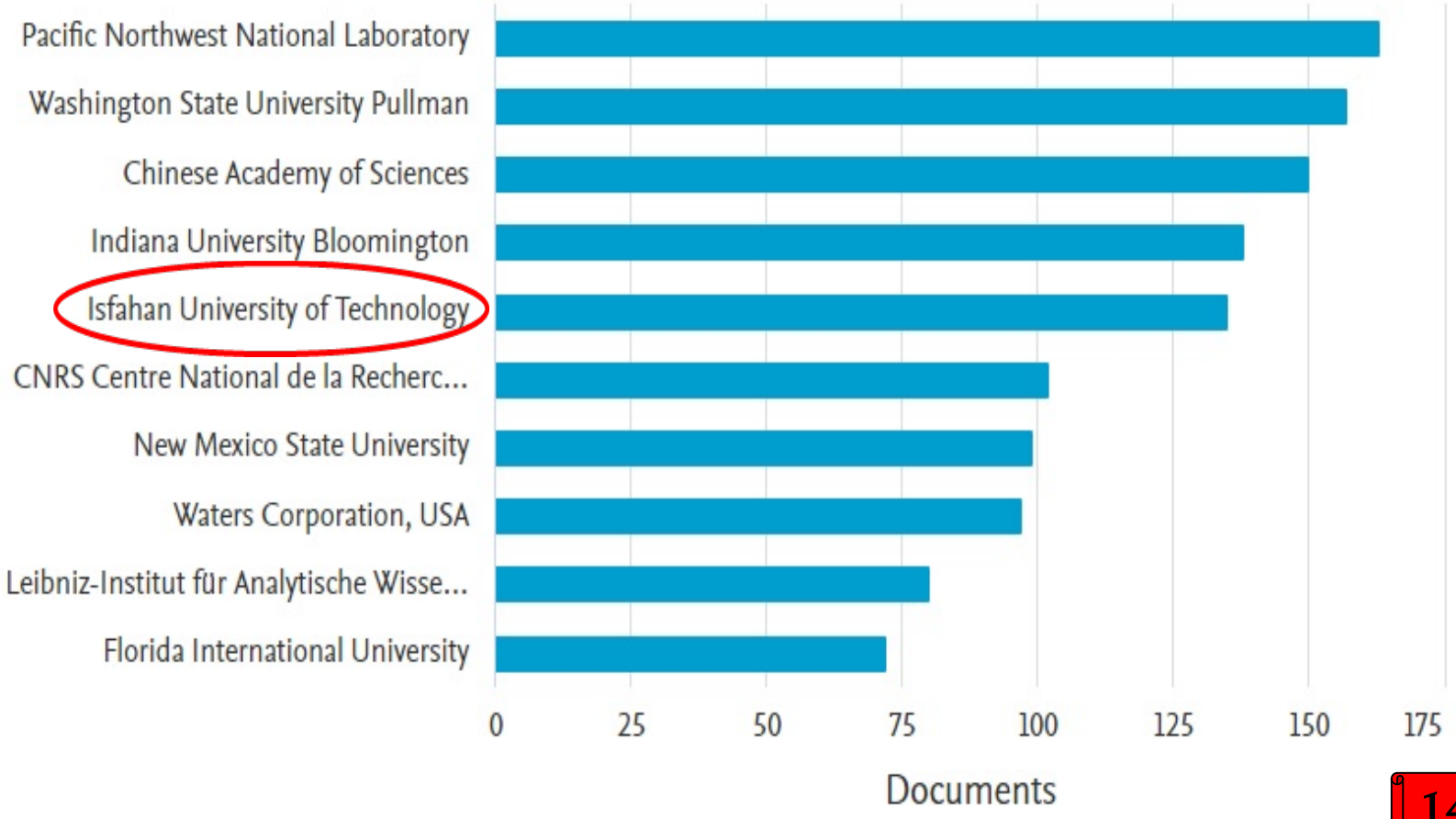
Publication



Publication

Documents by affiliation

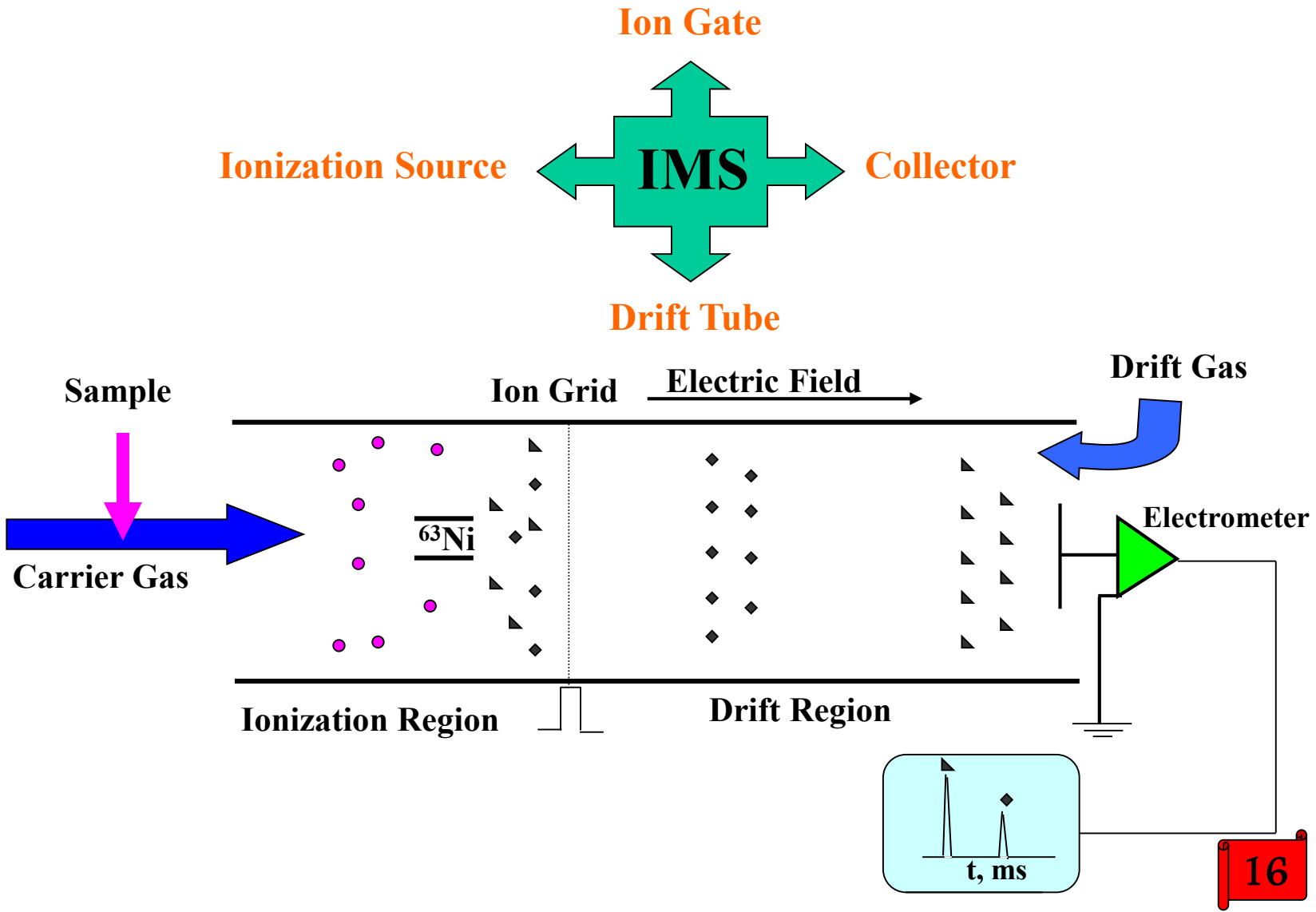
Compare the document counts for up to 15 affiliations.



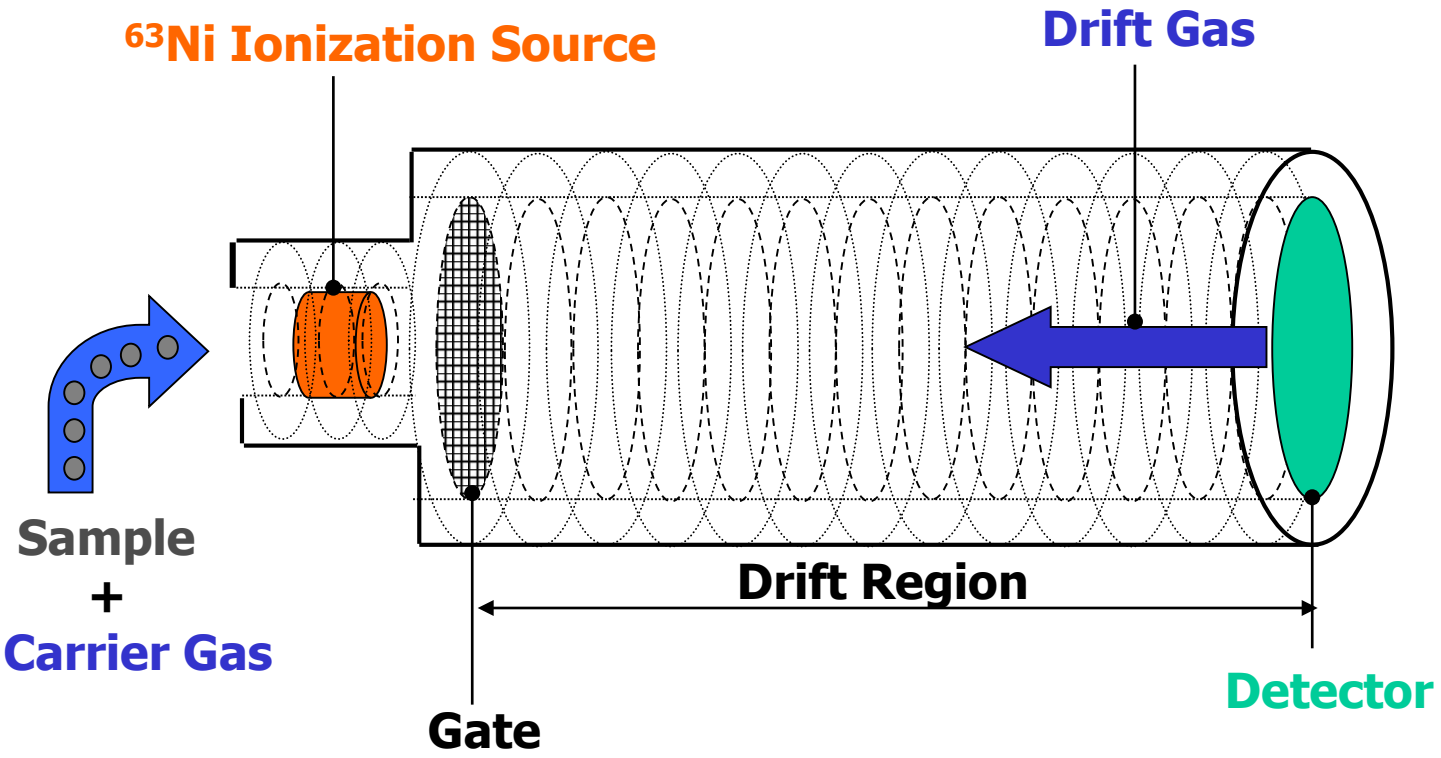
Publication

❖ ***Who is publishing in the ion mobility field?***

Ion Mobility Spectrometry (IMS)



Ion Mobility Spectrometry (IMS)



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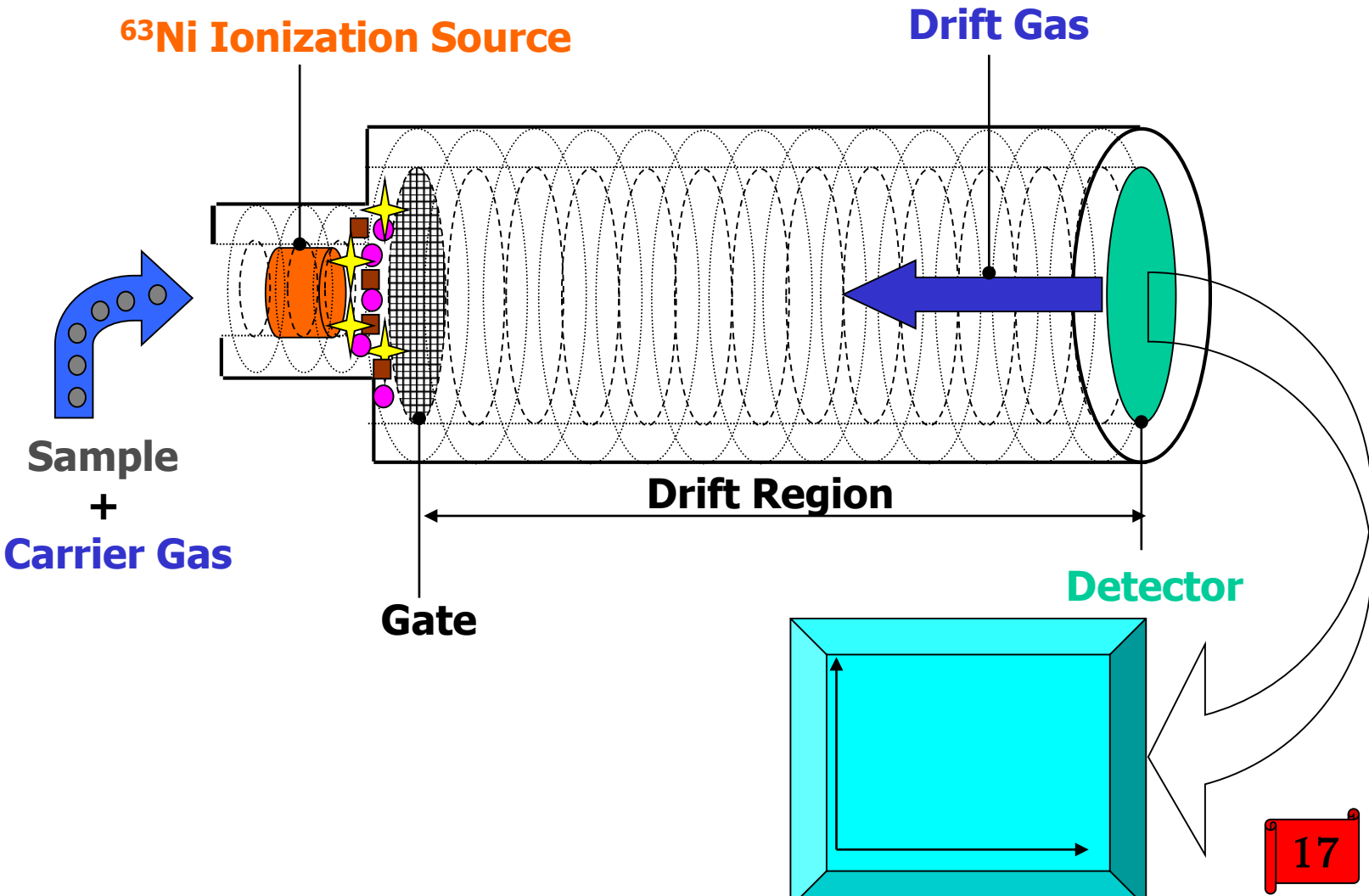
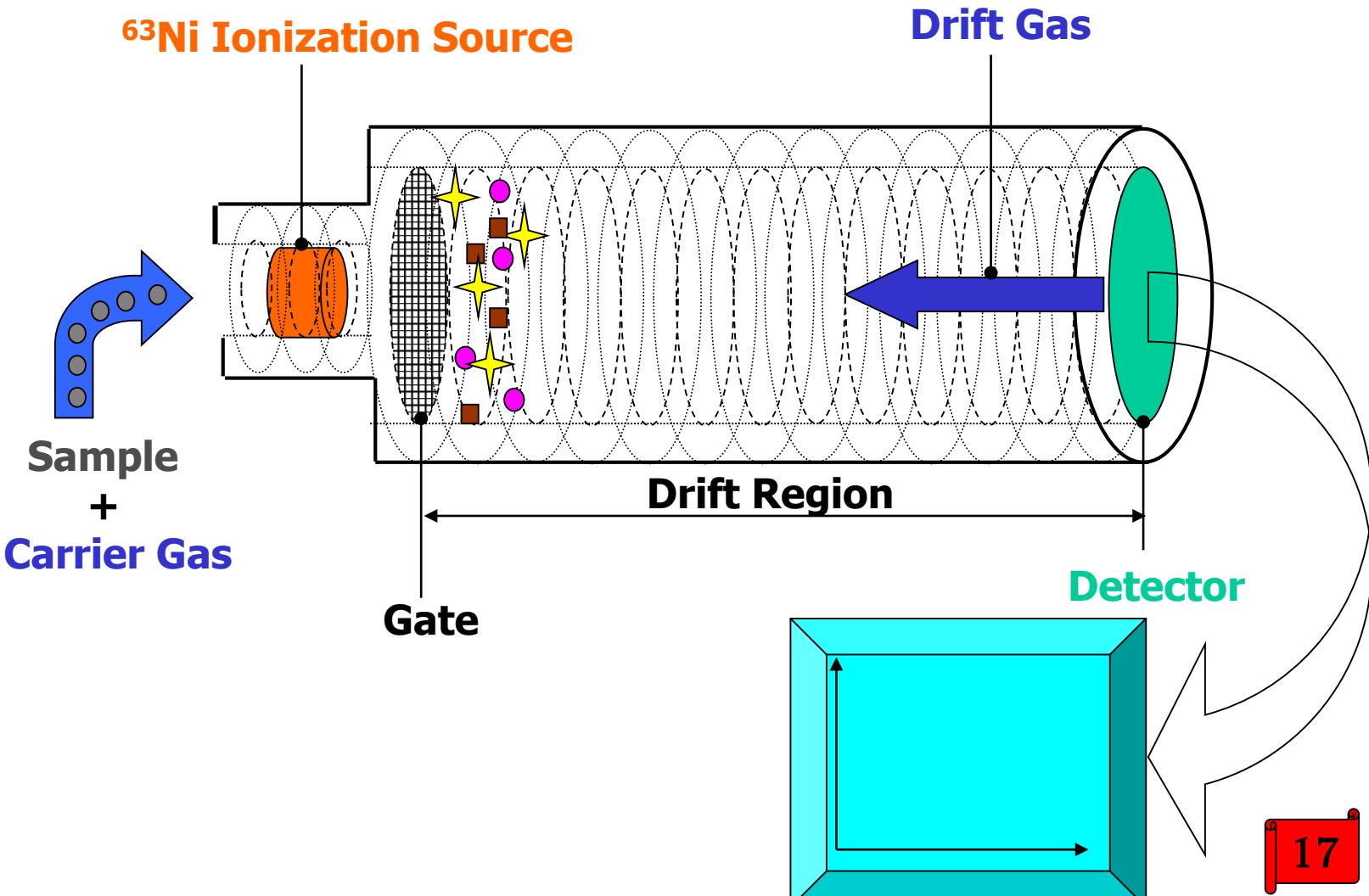


Ion Mobility Spectrometry (IMS)



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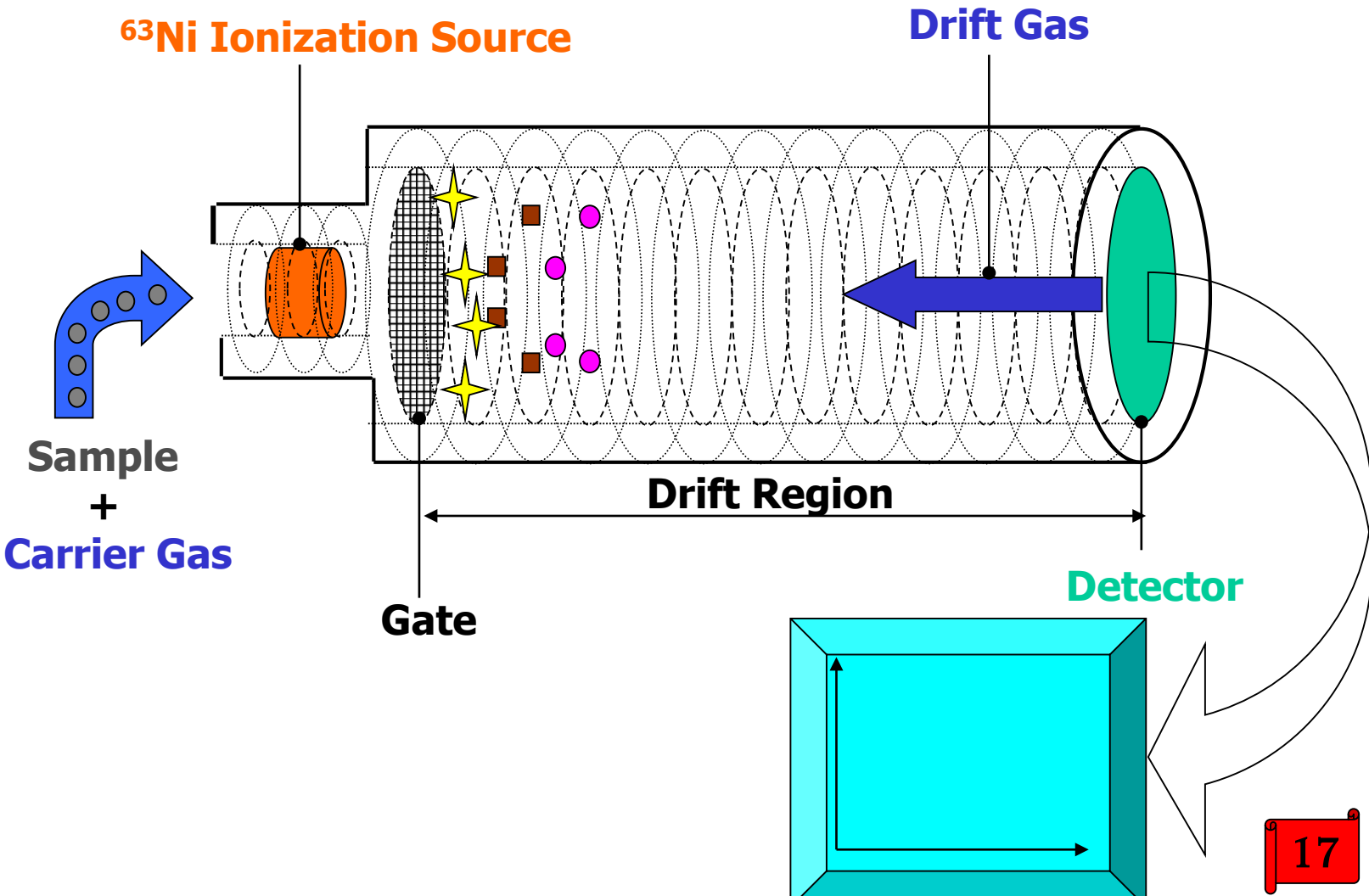
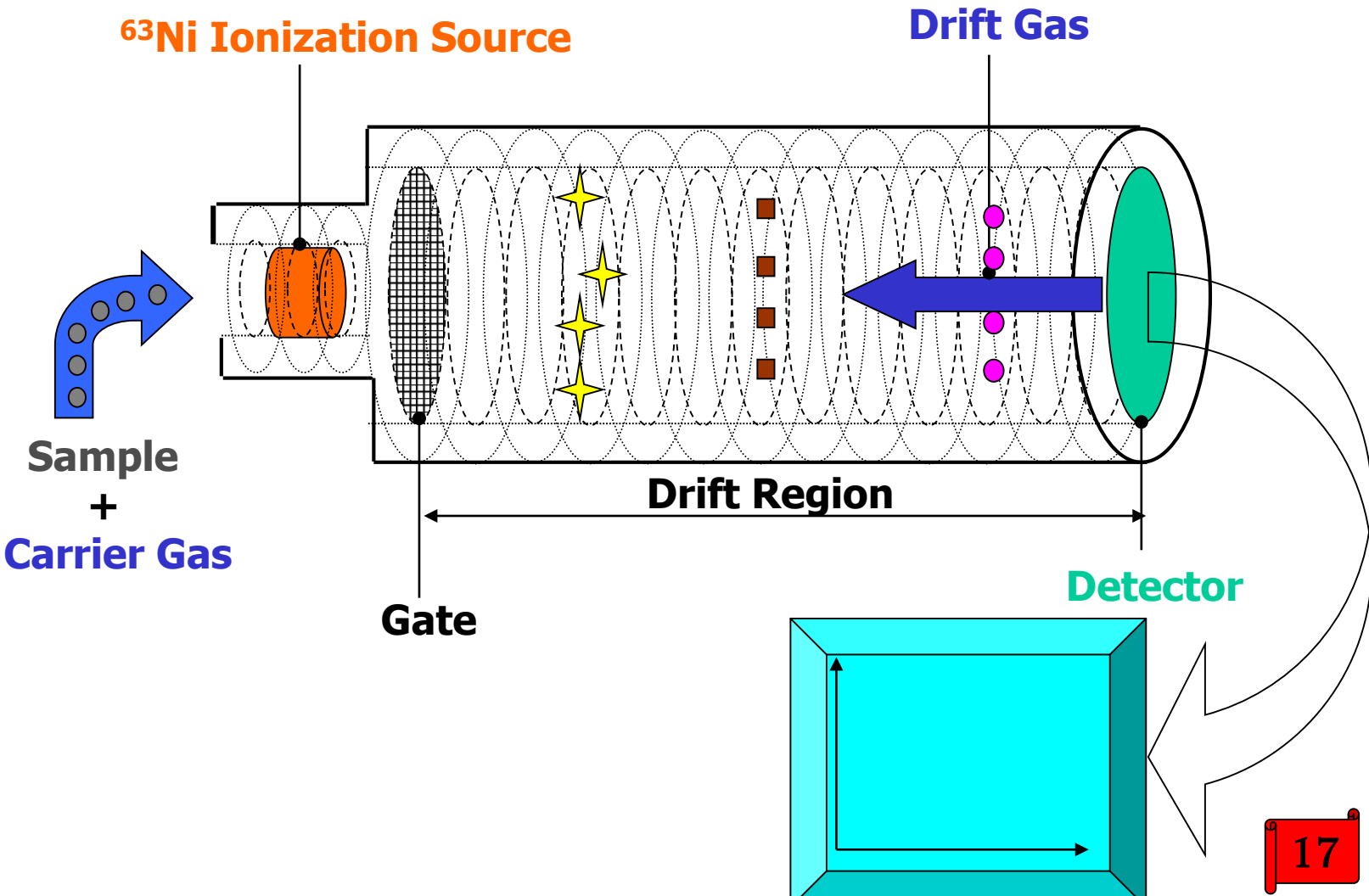
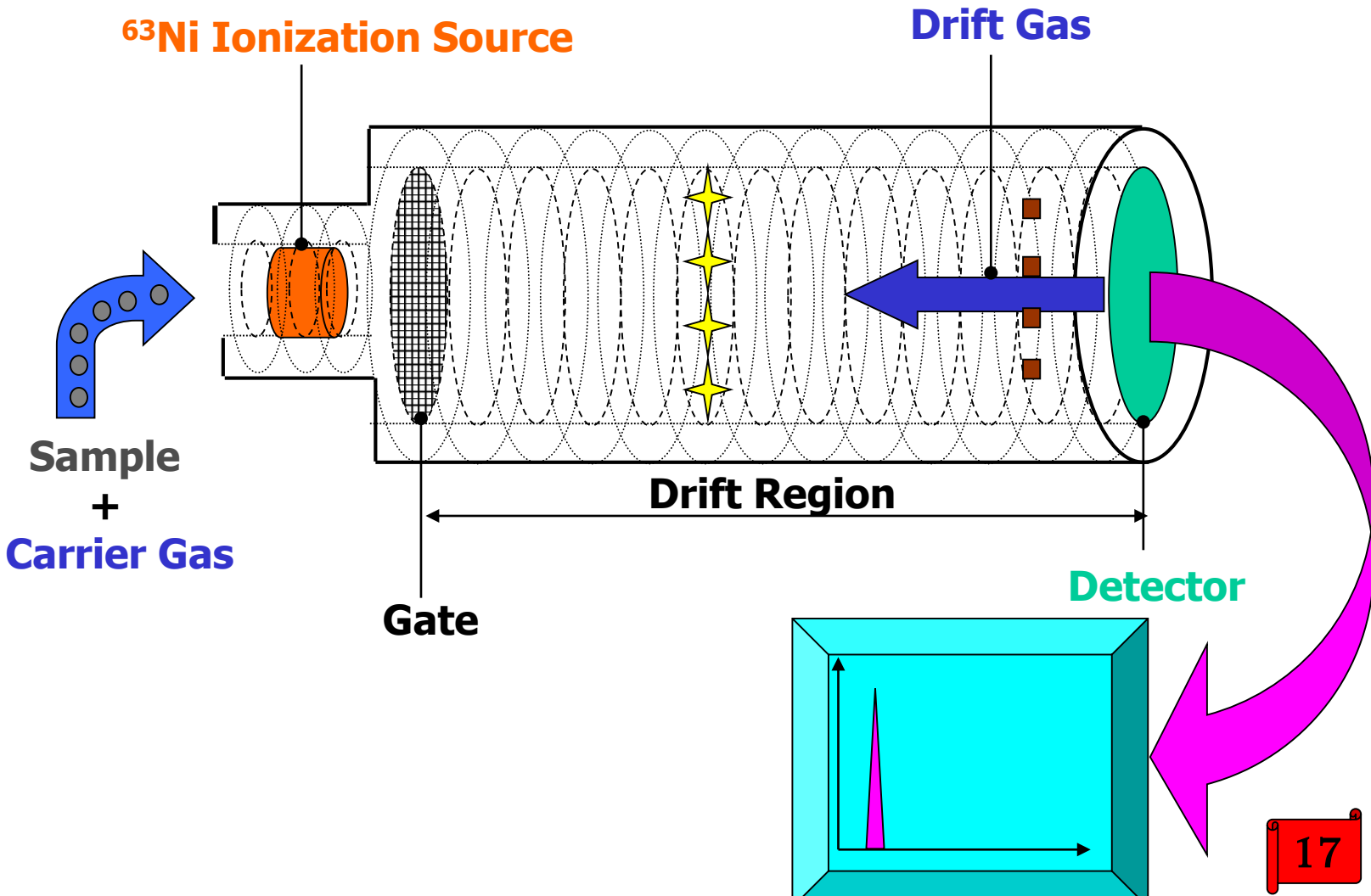


Ion Mobility Spectrometry (IMS)



Ion Mobility Spectrometry (IMS)



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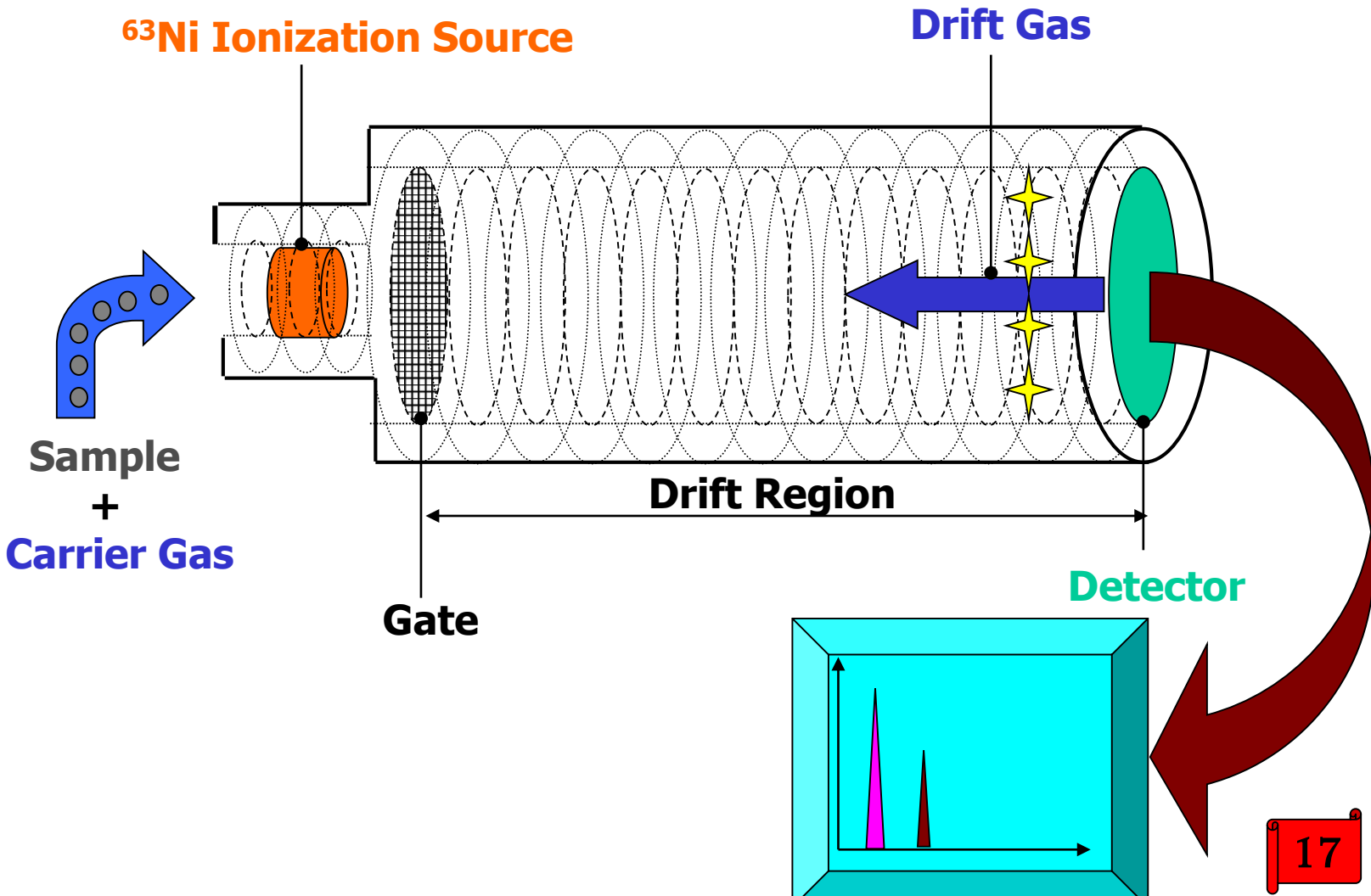
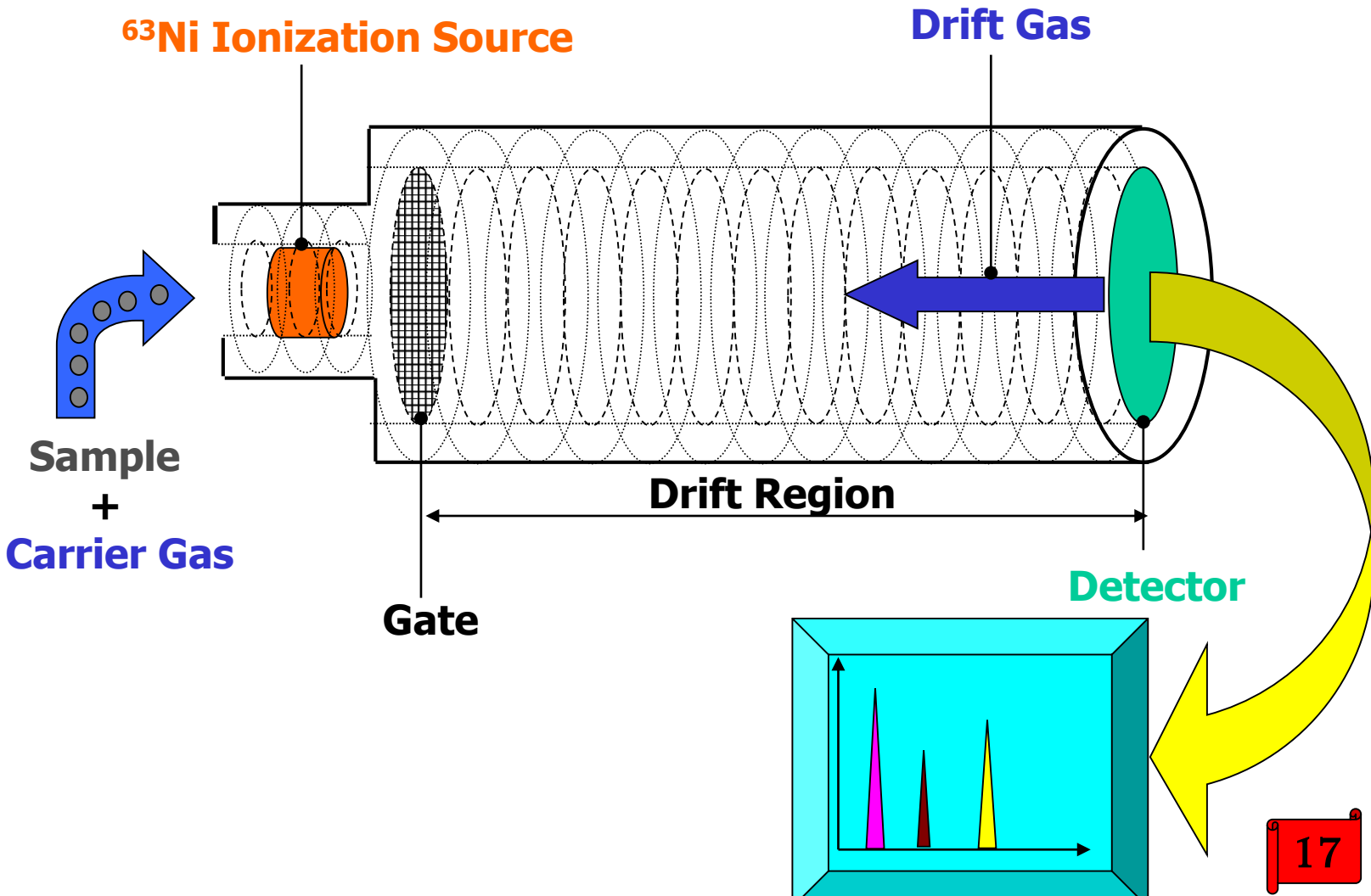


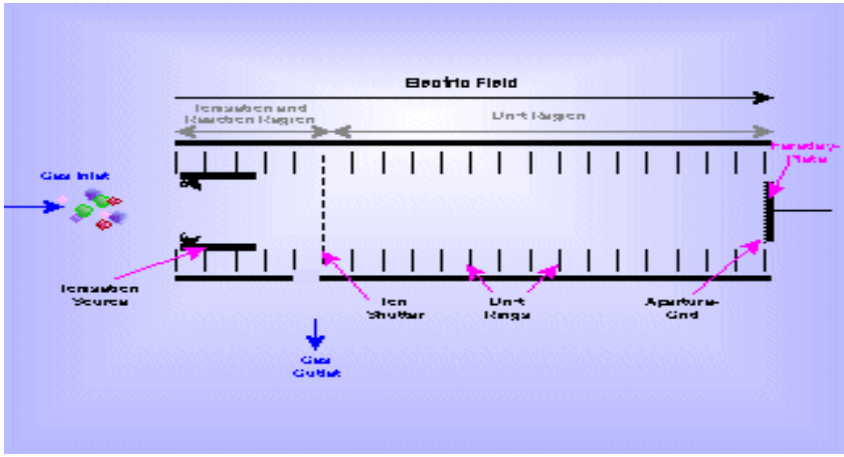
Ion Mobility Spectrometry (IMS)



Ion Characterization

The separation of ions is dependent to:

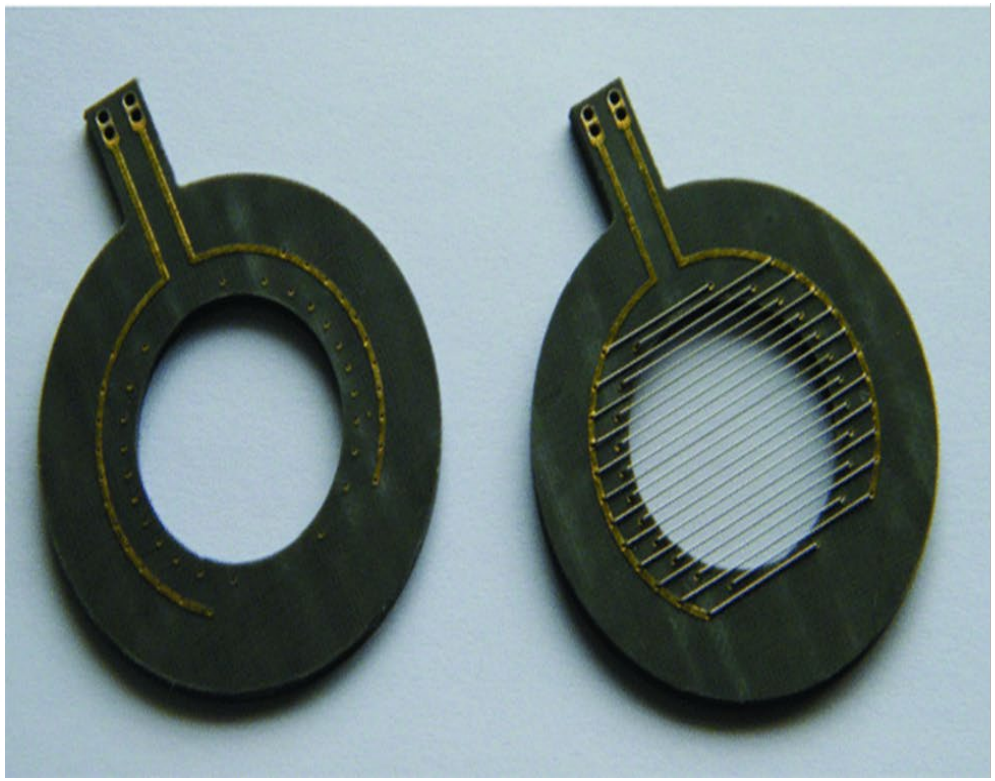
A) The ion mass
B) The ion charge
C) The ion shape

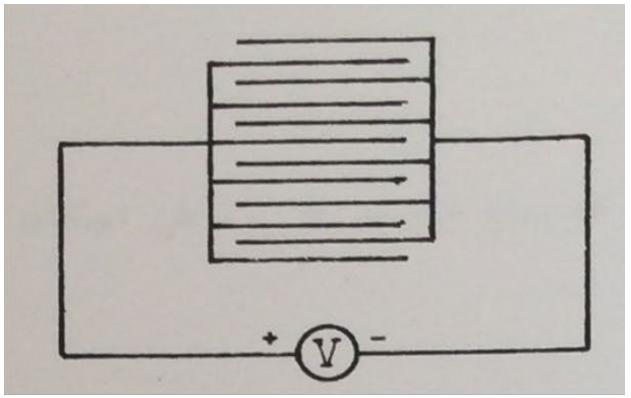


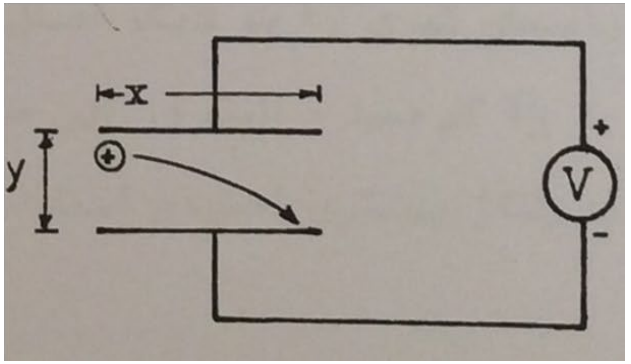
$$\left.\begin{aligned} K &= \frac{\upsilon}{\mathrm{E}} \\ \upsilon &= \frac{\mathrm{d}}{\mathrm{t}} \end{aligned}\right\} \quad K = \frac{\mathrm{d}}{\mathrm{t} \times \mathrm{E}}$$

$$K_o = K \times \left(\frac{273}{\mathrm{T}}\right) \times \left(\frac{\mathrm{P}}{760}\right)$$

Shutter Grid







IMS *vs* Mass Spectrometry

The advantage of IMS related to mass spectrometry (MS) is that IMS can be used for separation of ions under atmospheric pressure, and this ability is achieved on the basis of the ion shape in addition to the ion mass and charge, which are used in MS.

	Aspect compared	IMS	MS
Advantages of IMS	Cost	Low	High
	Portability	High	Medium
	Ease Of Use	Easy	Complex
	Maintenance	Low	High
	Speed	High	Medium
Disadvantages of IMS	Sensitivity	Medium	High
	Selectivity	Low	High
	Sample introduction	Medium	Medium
	Applicability	Limited	Broad

Trends in Analytical Chemistry, Vol. 30, 2011, 677-690.

Ionization Sources

Gas phase

- *Radioactive Source (^{63}Ni)*
- *Corona Discharge (CD)*
- *Chemical Flame*

Liquid phase

- *Photo Ionization (PI)*
- *Electrospray Ionization (ESI)*

Solid, liquid and gaseous phase

- *Low Temperature Plasma (LTP)*

Ionization Mechanism

Stability, releability, without an extra power source.

$$N_2 + e^- \text{ (primary)} \longrightarrow N_2^+ + e^- \text{ (primary)} + e^- \text{ (secondary)}$$

$$N_2^+ + 2N_2 \longrightarrow N_4^+ + N_2$$

$$N_4^+ + H_2O \longrightarrow 2N_2 + H_2O^+$$

$$H_2O^+ + H_2O \longrightarrow OH^- + H_3O^+$$

$$H_3O^+ + H_2O + N_2 \leftrightharpoons (H_2O)_2H^+ + N_2$$

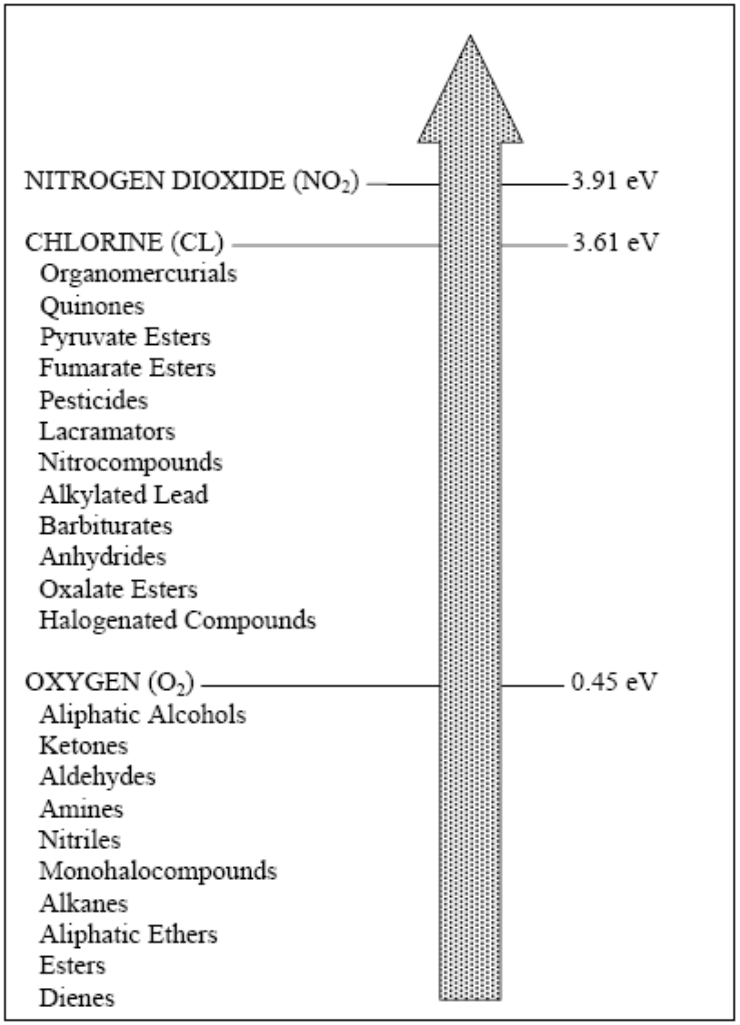
$$H^+(H_2O)_n + M \leftrightharpoons MH^+(H_2O)_n^* + Z \leftrightharpoons MH^+(H_2O)_{n-1} + H_2O + Z$$

$$M + O_2^-(H_2O)_n \longrightarrow MO_2^-(H_2O)_{n-x} + xH_2O$$

Sample + negative reactant ion → Product ion + water

Selectivity Parameter

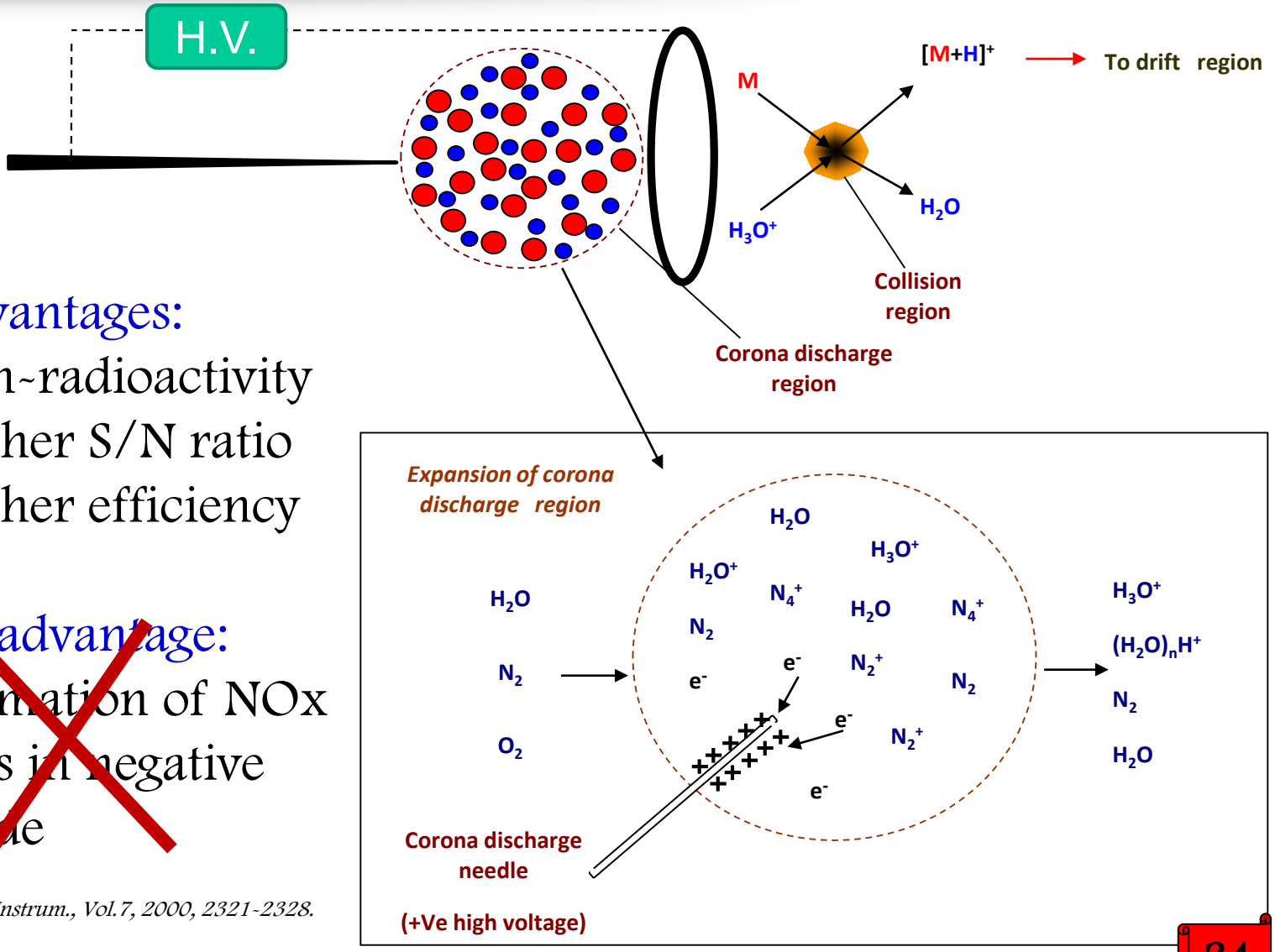
Electron Affinity (EA)



Proton Affinity (PA)

CHEMICAL FAMILY	PROTON AFFINITY OF REPRESENTATIVE CHEMICAL	
Aromatic Amines	930 kJ/mole	Pyridine
Amines	899.0 kJ/mole	Methyl Amine
Phosphorous compounds	890.6 kJ/mole	trimethylphosphate
Sulfoxides	884.4 kJ/mole	Dimethyl sulfoxide
	853.6 kJ/mole	Ammonia
Ketones	832.7 kJ/mole	2-Pentanone
Esters	821.6 kJ/mole	Methyl Acetate
Alkenes	805.2 kJ/mole	1-Hexene
Alcohols	789.2 kJ/mole	Butanol
Aromatics	750.4 kJ/mole	Benzene
	691 kJ/mole	Water
Alkanes	543.5 kJ/mole	Methane

Corona Discharge Ionization



Advantages:

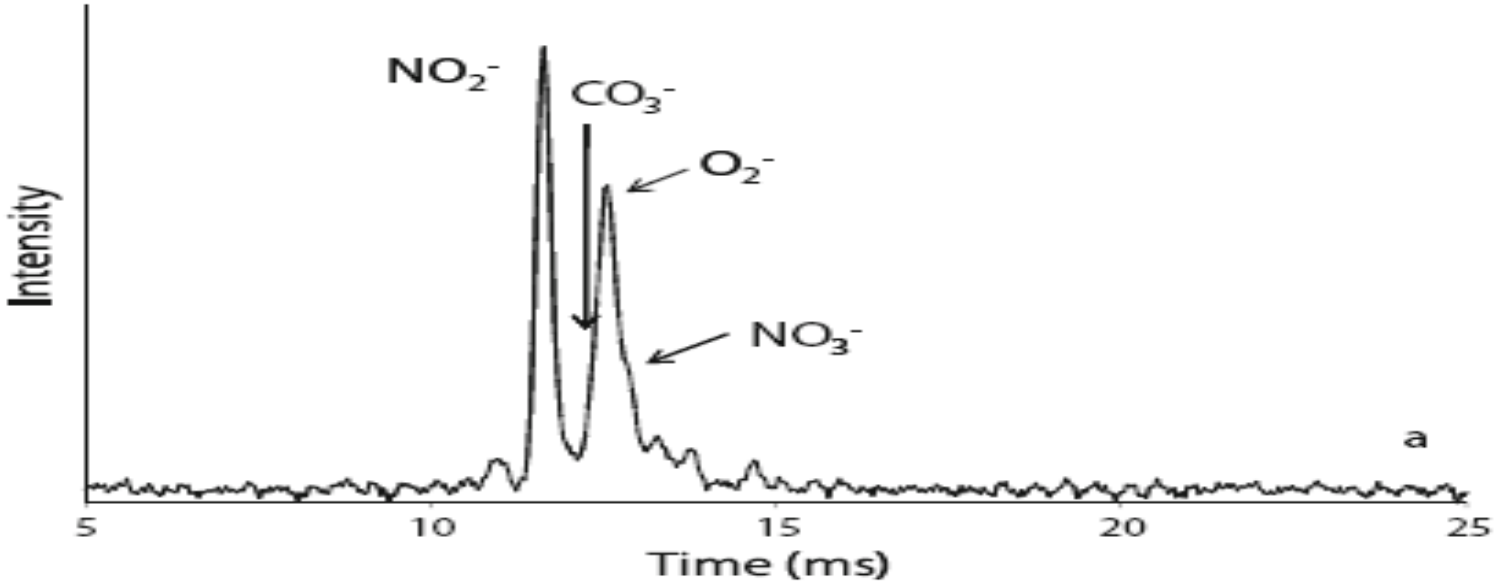
Non-radioactivity
Higher S/N ratio
Higher efficiency

Disadvantage:

Formation of NOx ions in negative mode

Rev. Sci. Instrum., Vol.7, 2000, 2321-2328.

Negative CD–IMS



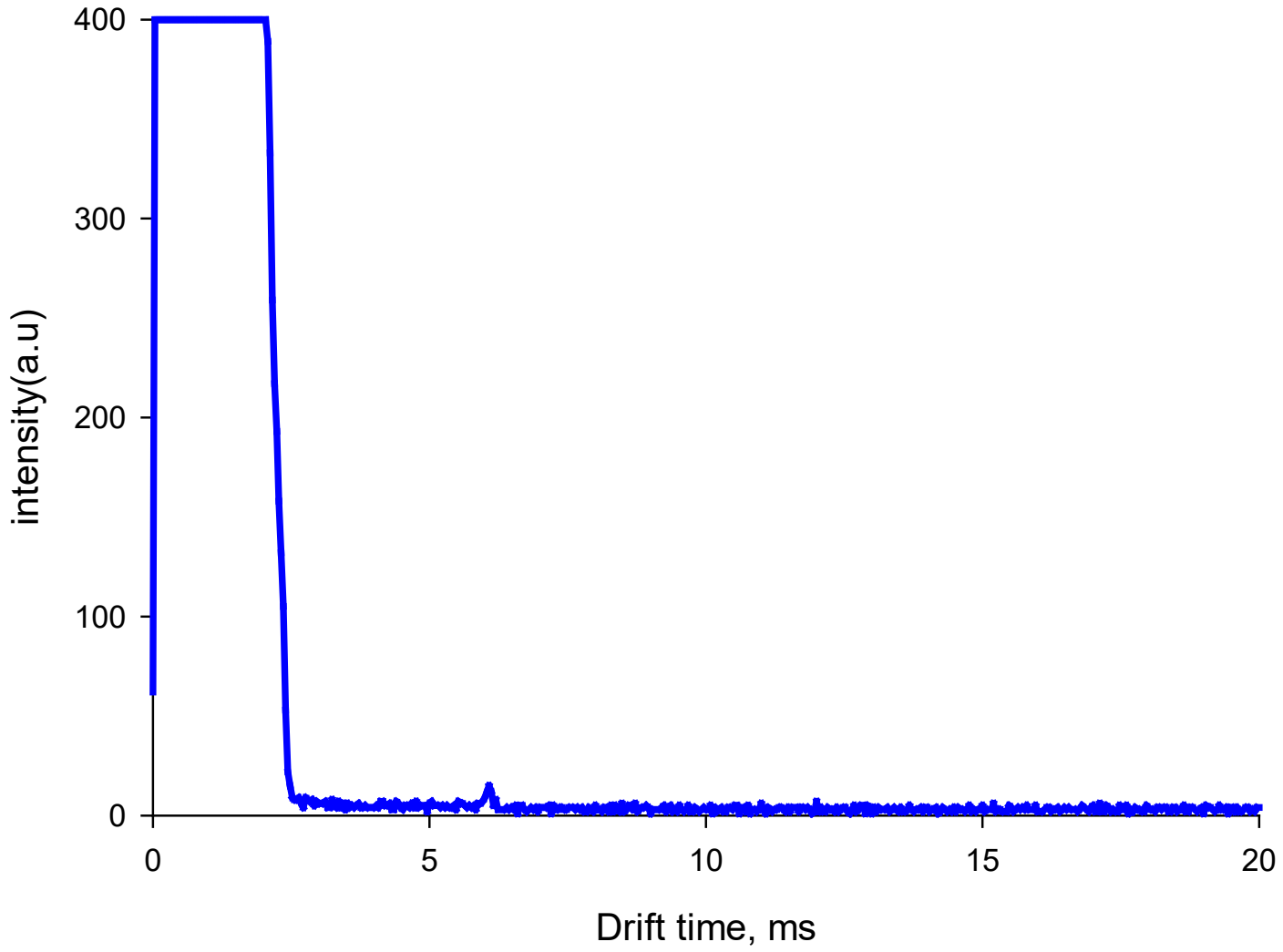
NO_X cluster ions have very high electron affinities (~ 3.9 eV) quenching the product ions.

It is impossible to analyze these ions themselves in a sample

Their signals may have overlapping with other peaks.

NO_X^- can joint to the analyte, making difficult to interpret the more complex mass or ion mobility spectra.

Negative CD–IMS Background



Novel Design for Negative Corona Discharge


قوه قضائیه

سازمان ثبت اسناد و املاک کشور

گواهی نامه ثبت اختراع

۰۳۸۶۰۹ الف/۸۹

مشخصات مالک:
محمد تقی جعفری به شماره ملی ۶۲۳۹۹--۵۹۹ به نشانی اصفهان- دانشگاه صنعتی اصفهان- دانشکده شیمی کد پستی ۸۴۱۵۶۸۳۱۱۱ تابعیت جمهوری اسلامی ایران

مشخصات مخترع:
محمد تقی جعفری به شماره ملی ۶۲۳۹۹--۵۹۹ به نشانی اصفهان-دانشگاه صنعتی اصفهان-دانشکده شیمی کد پستی ۸۴۱۵۶۸۳۱۱۱ تابعیت جمهوری اسلامی ایران

عنوان اختراع: طراحی منبع یونیزاسیون تخلیه کرونا در مد منفی بدون مزاحمت یون های NOx

طبقه بندی بین المللی:

حق تقدم:

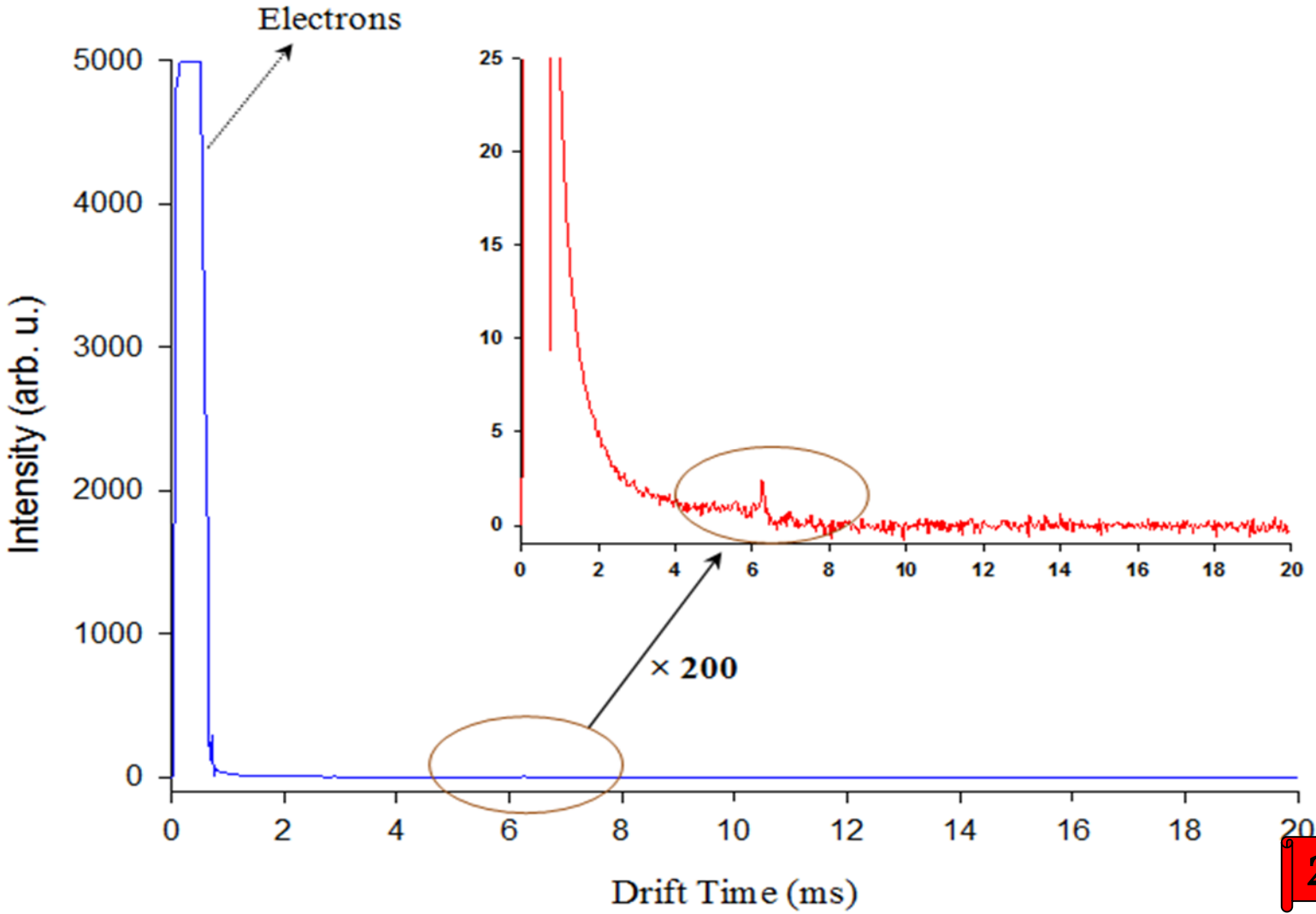
شماره و تاریخ اظهارنامه اصلی :　　محل ثبت:

مدت حمایت: ۲۰ سال از تاریخ ۱۳۹۱/۰۹/۰۶	شماره و تاریخ ثبت اظهارنامه: [illegible] - ۱۳۹۱/۰۹/۰۶	شماره و تاریخ ثبت اختراع: ۷۹۲۵۲ - ۱۳۹۲/۰۲/۰۳

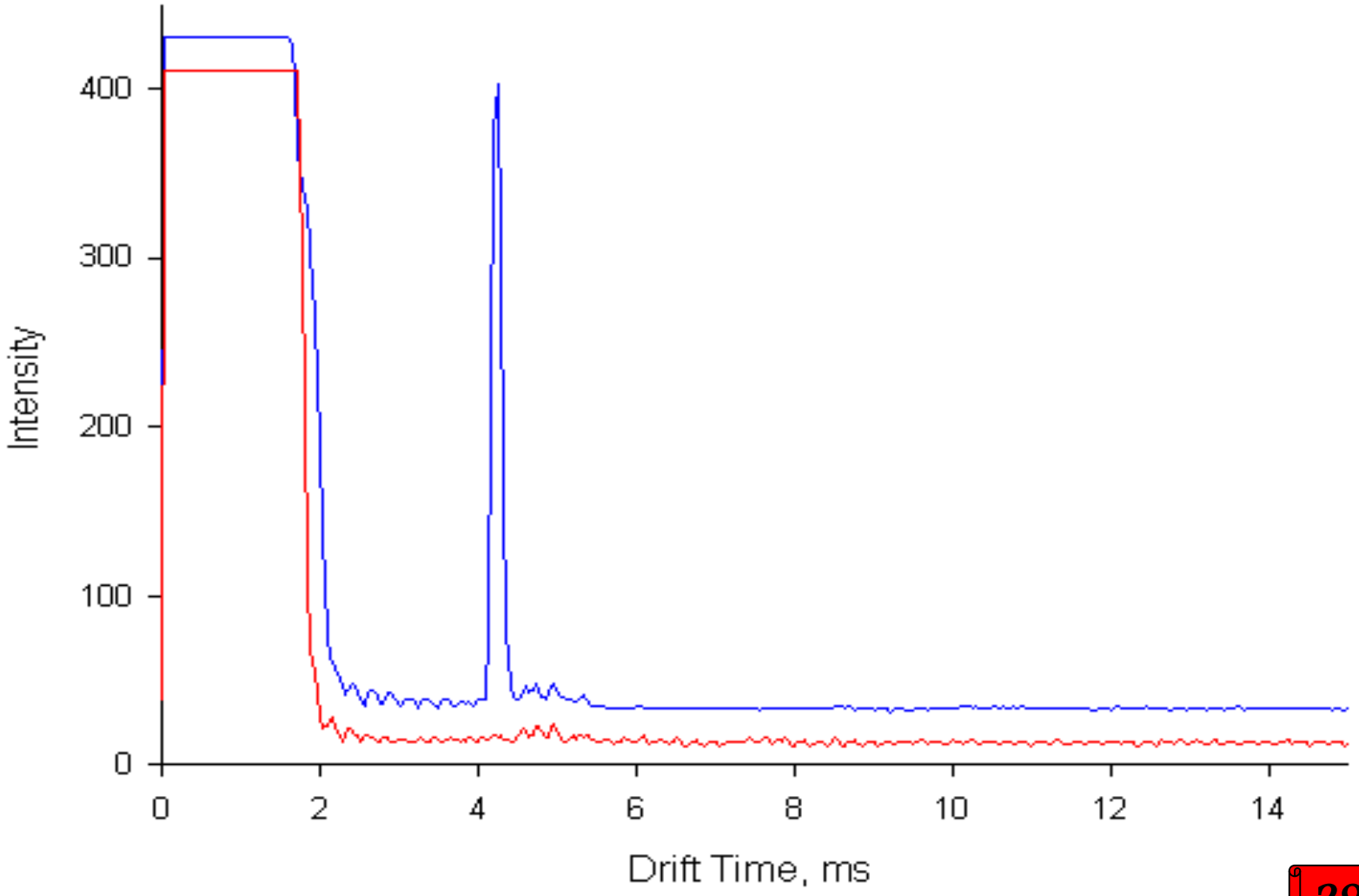
اداره کل مالکیت صنعتی
رئیس اداره ثبت اختراعات　مهرداد الیاسی　تاریخ:　امضاء:

* ضمائم گواهی نامه: توصیف ادعا، خلاصه توصیف، نقشه
** درصورت تعدد مخترعین، مالکین یا تغییرات، مراتب شرح مندرج در ظهر گواهی نامه می باشد.

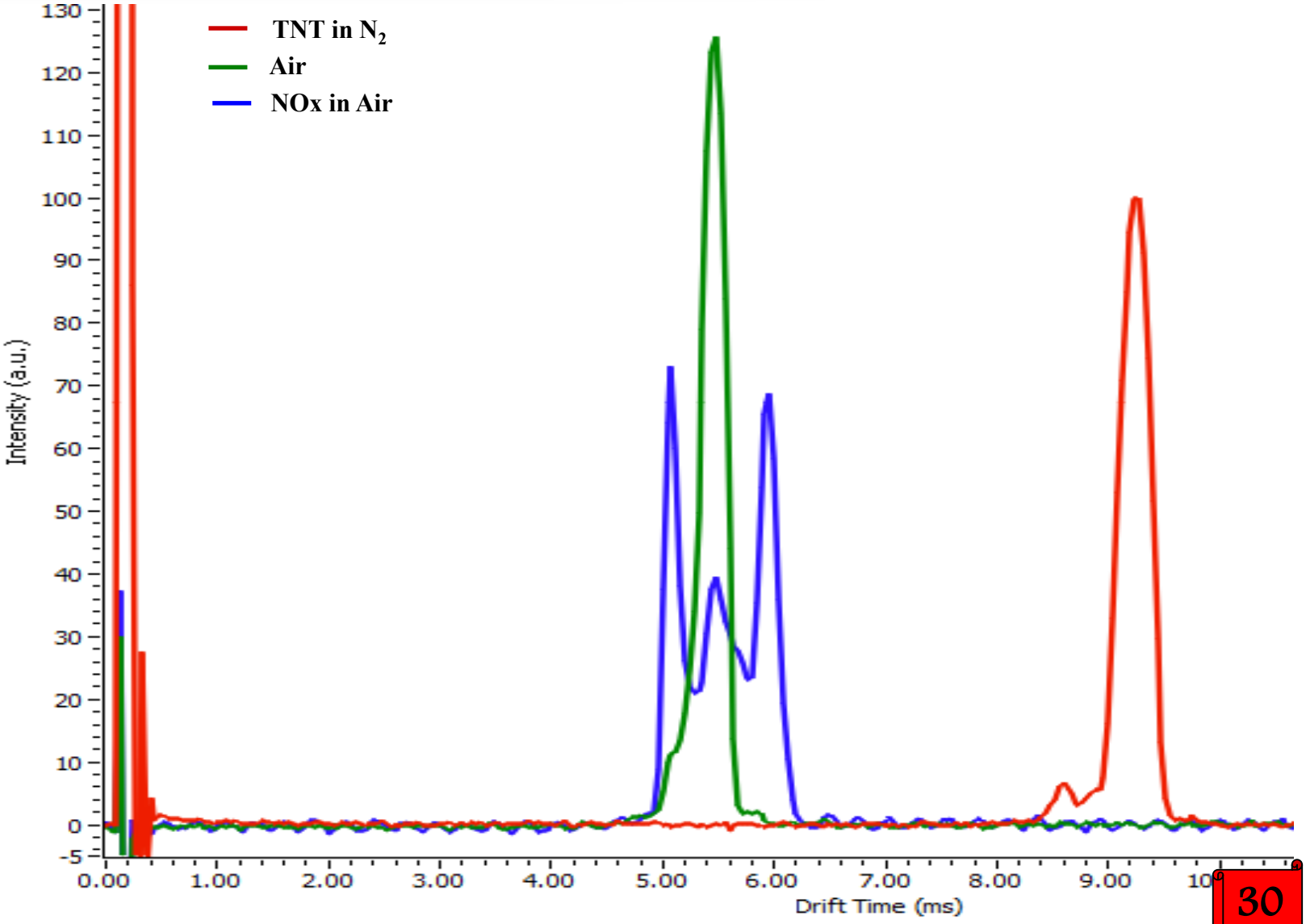
Negative CD–IMS Background



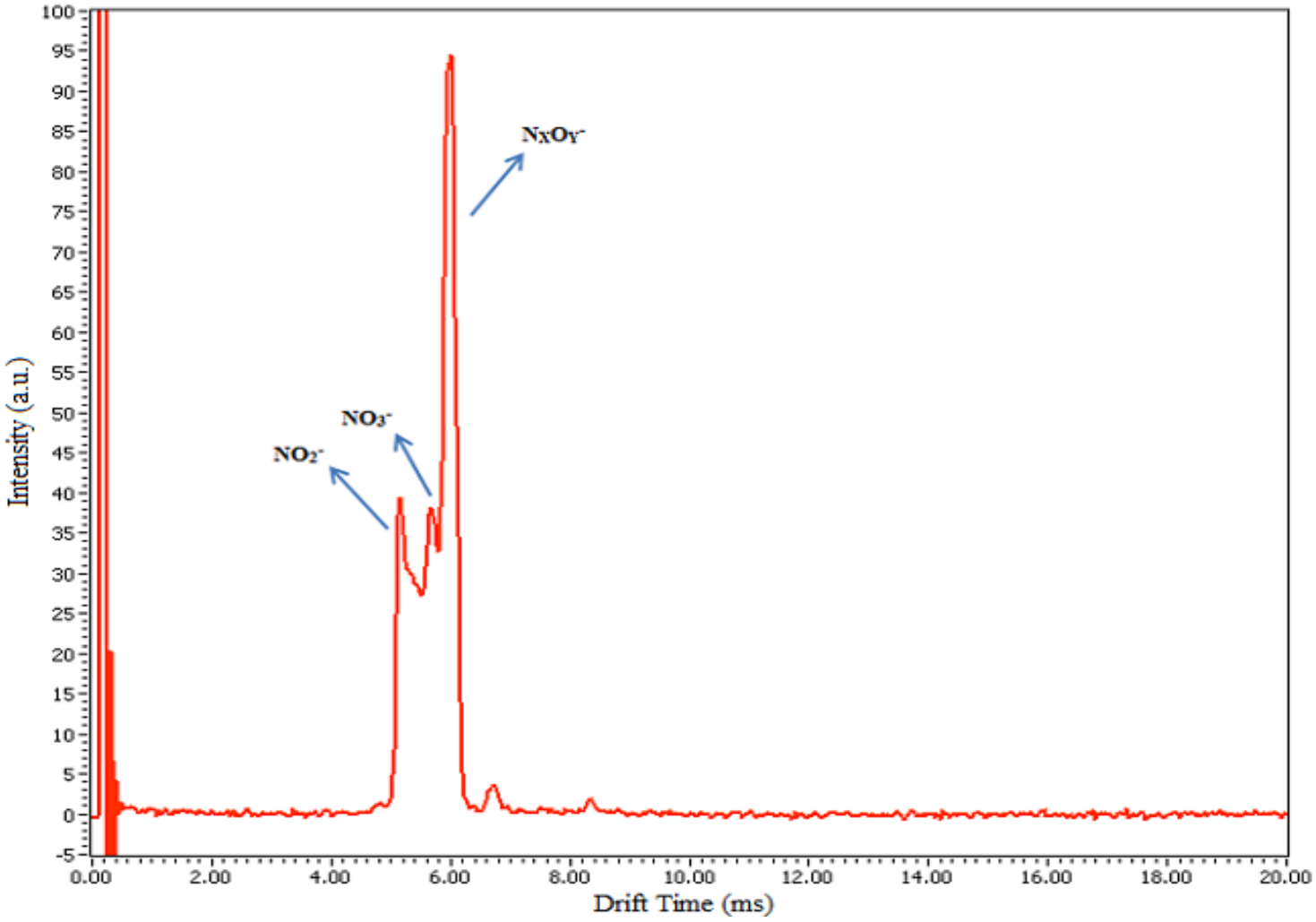
Oxygen Analysis by NCD~IMS



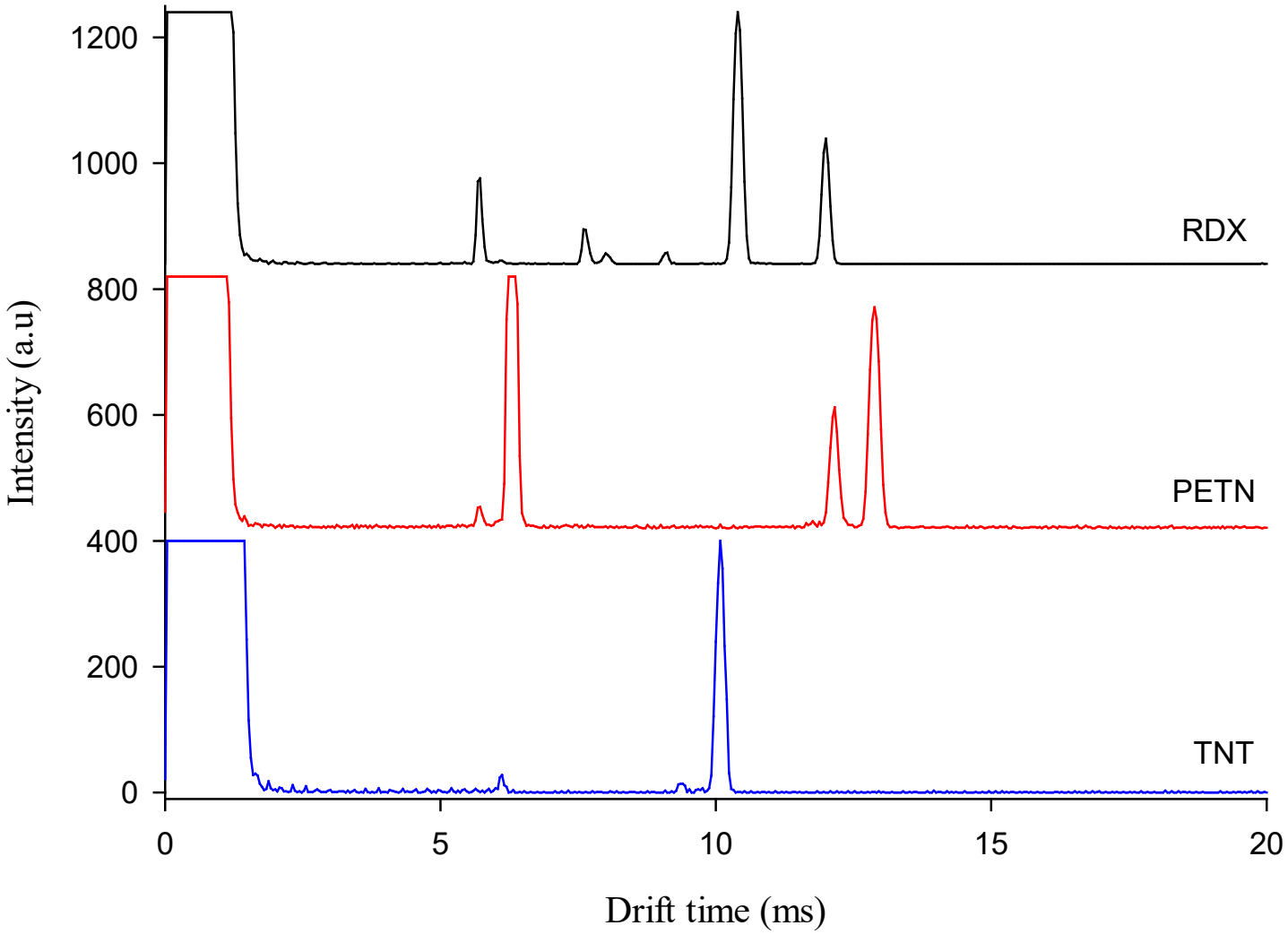
Novel Design of NCD-IMS



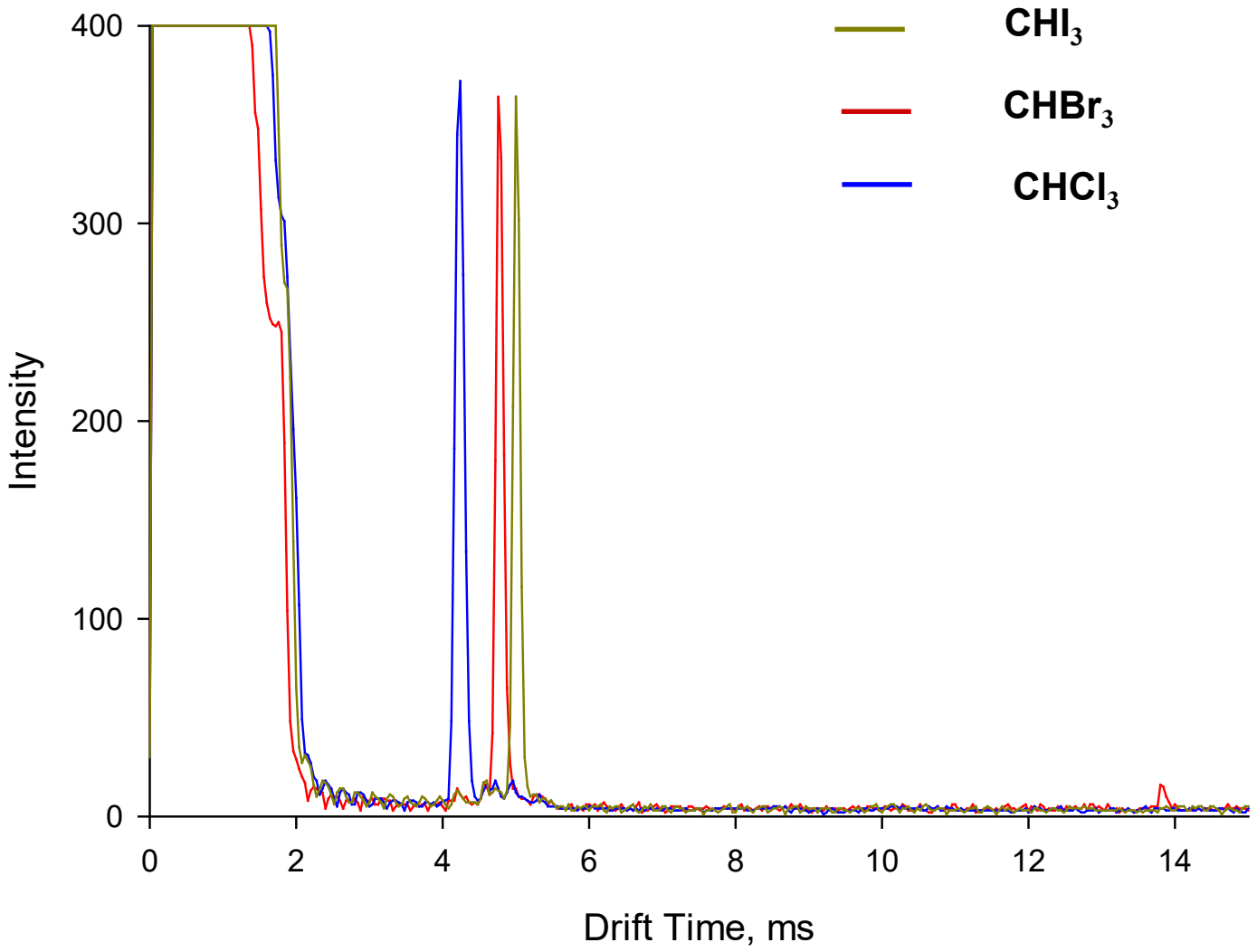
NOx analysis by NCD-IMS



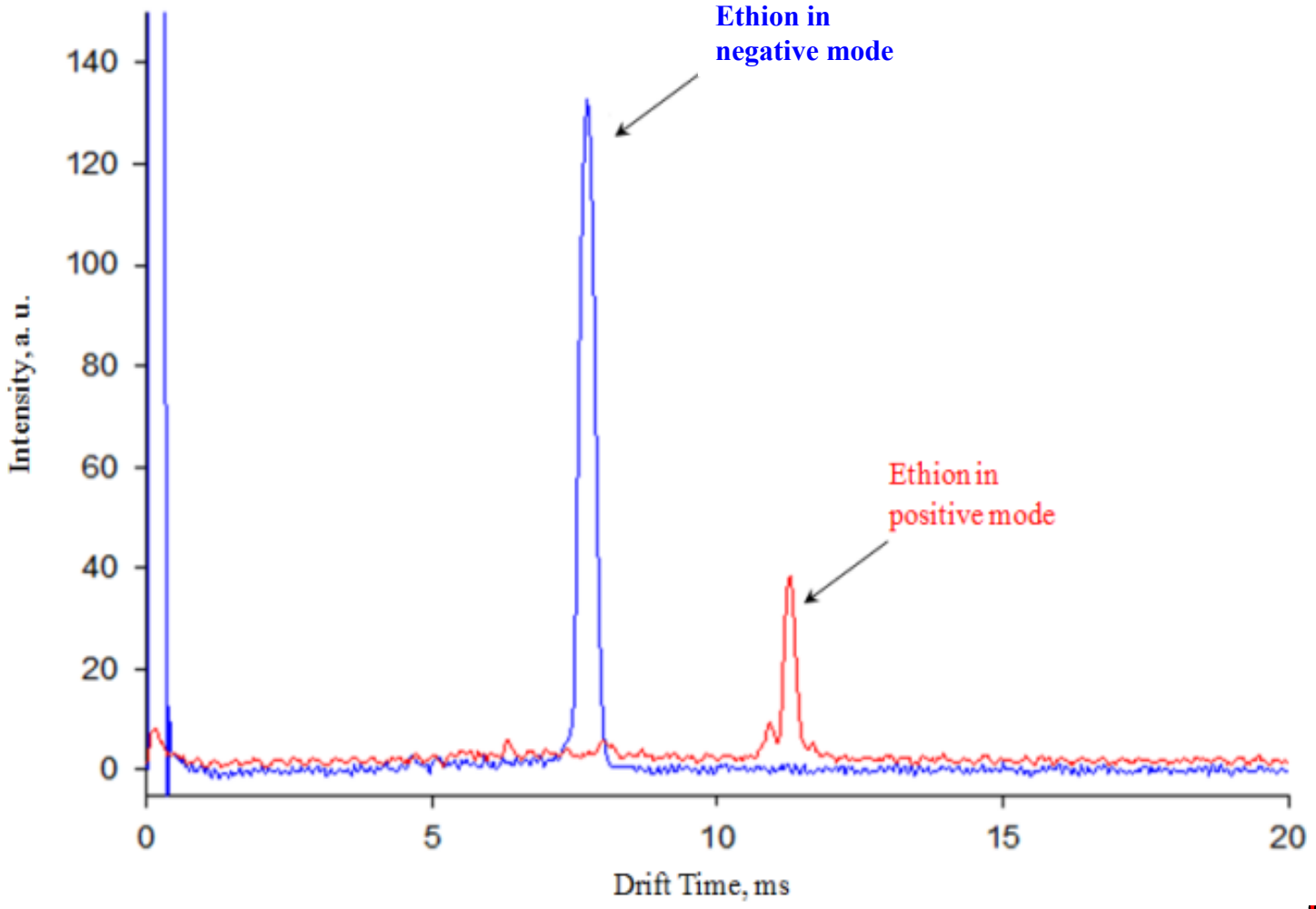
Mobility Spectra of Explosives



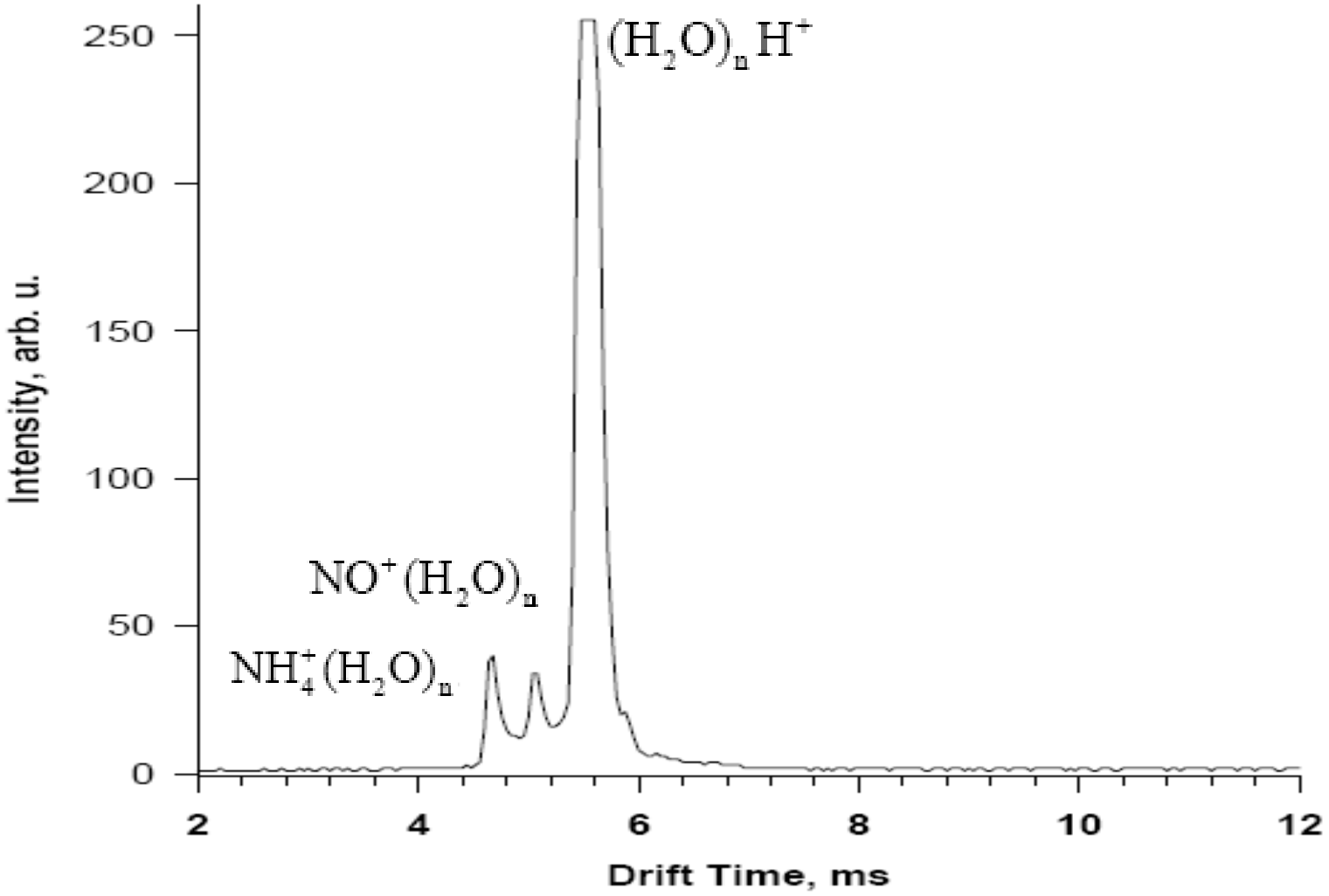
Mobility Spectra of Cl, Br, I



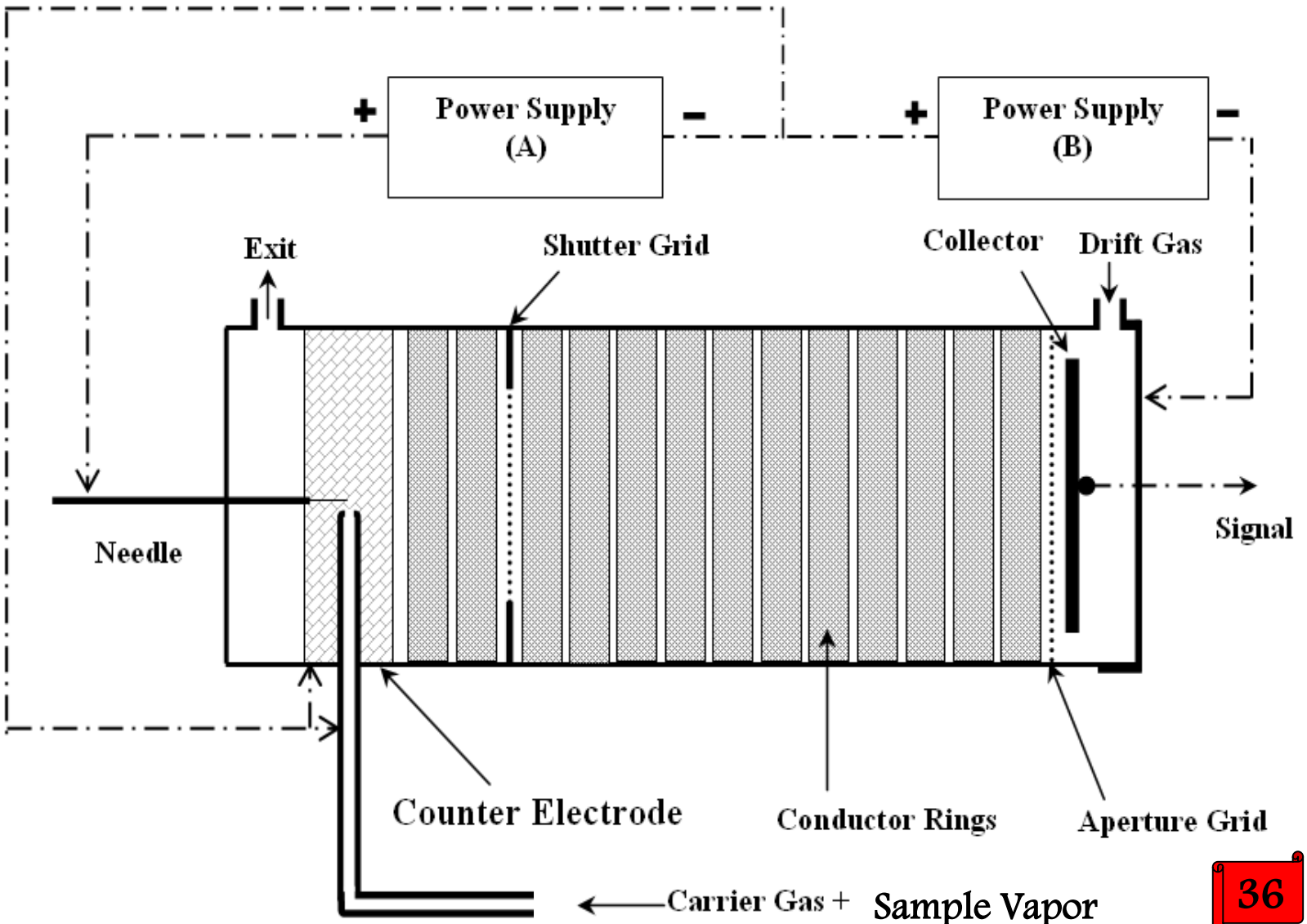
Mobility spectrum of Ethion in positive and negative



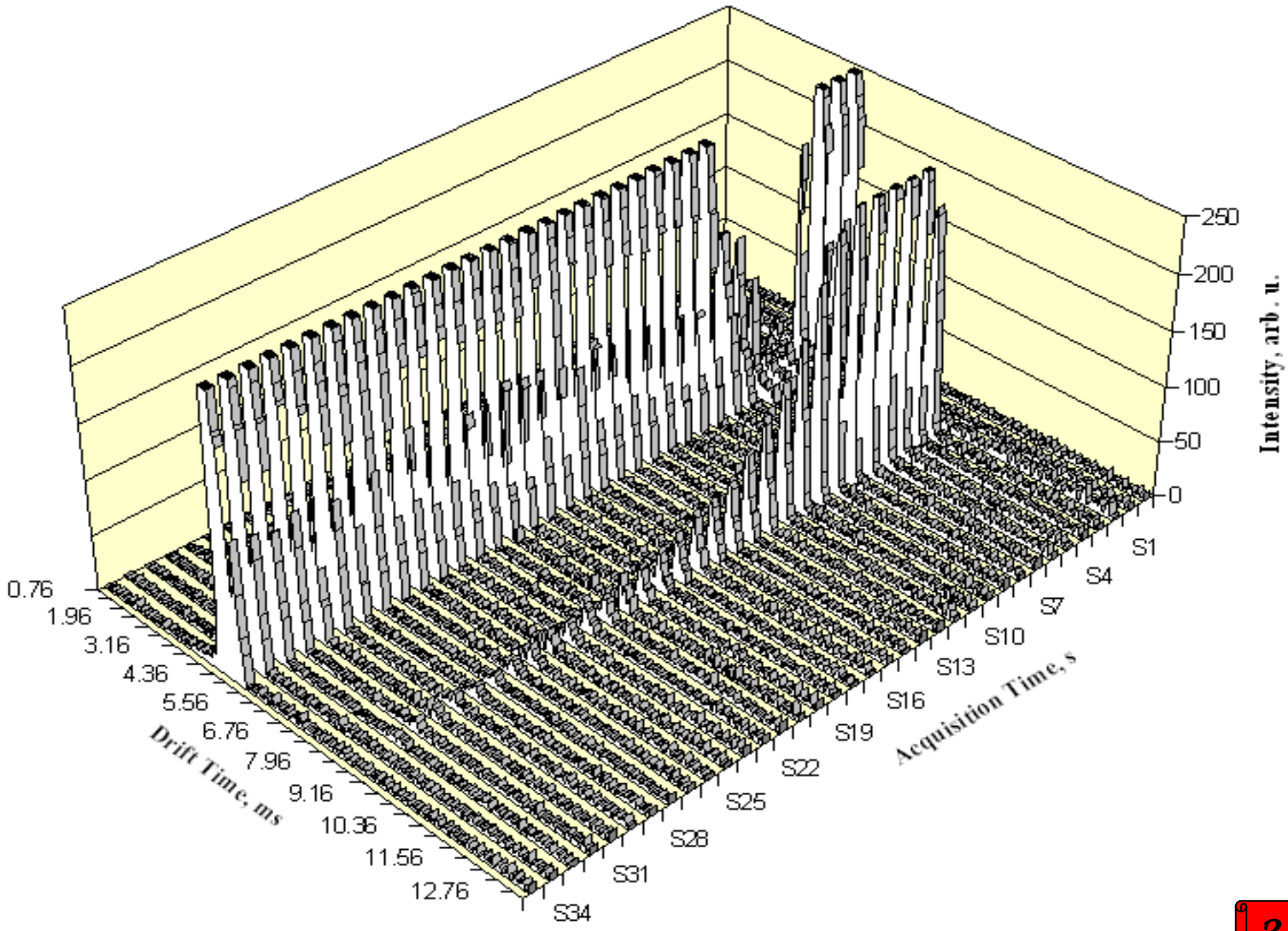
Positive Background Spectrum



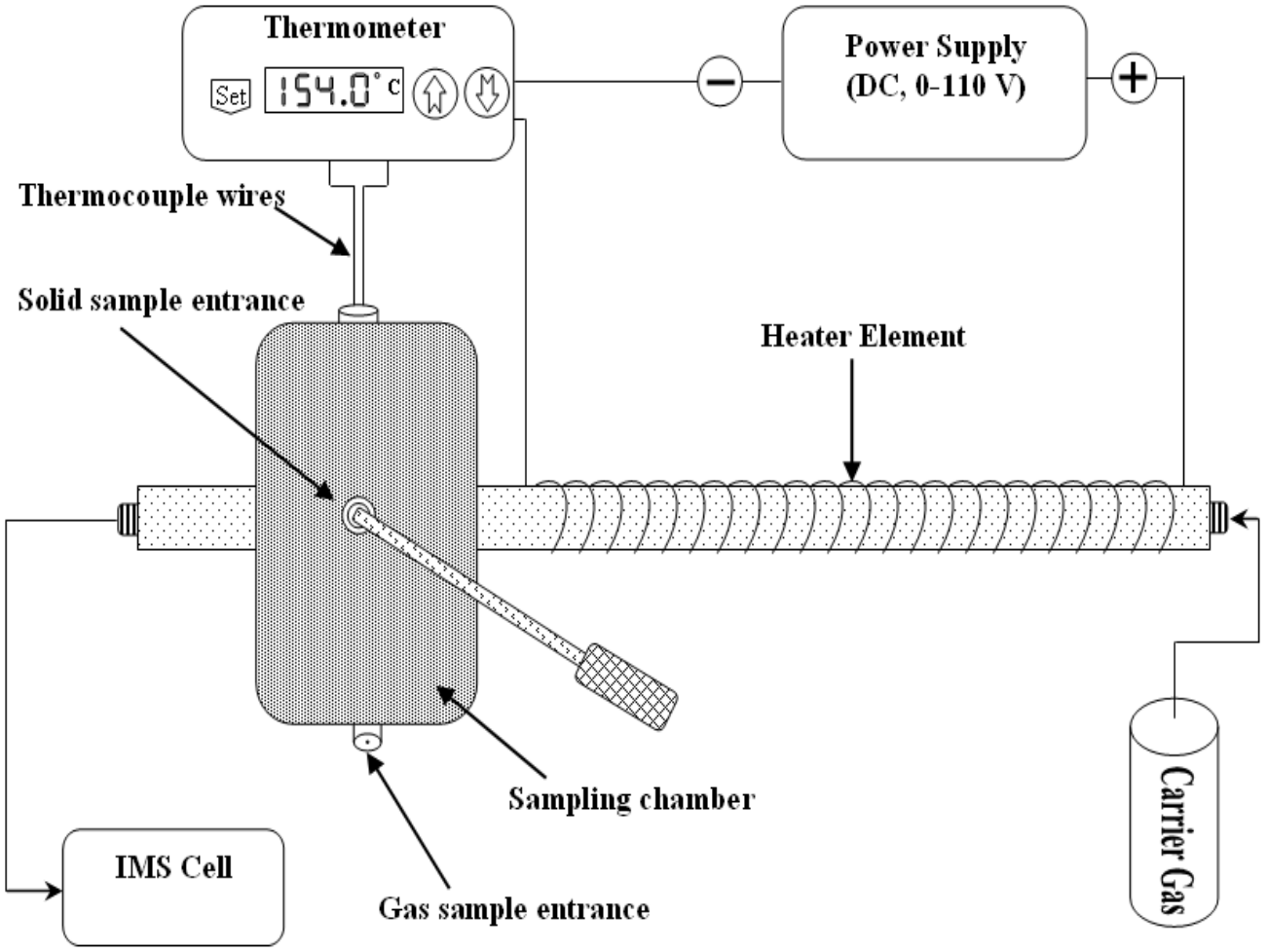
IMS Cell


+
Power Supply
(A)
-
+
Power Supply
(B)
-
Exit
Shutter Grid
Collector
Drift Gas
Needle
Signal
Counter Electrode
Conductor Rings
Aperture Grid
Carrier Gas +
Sample Vapor

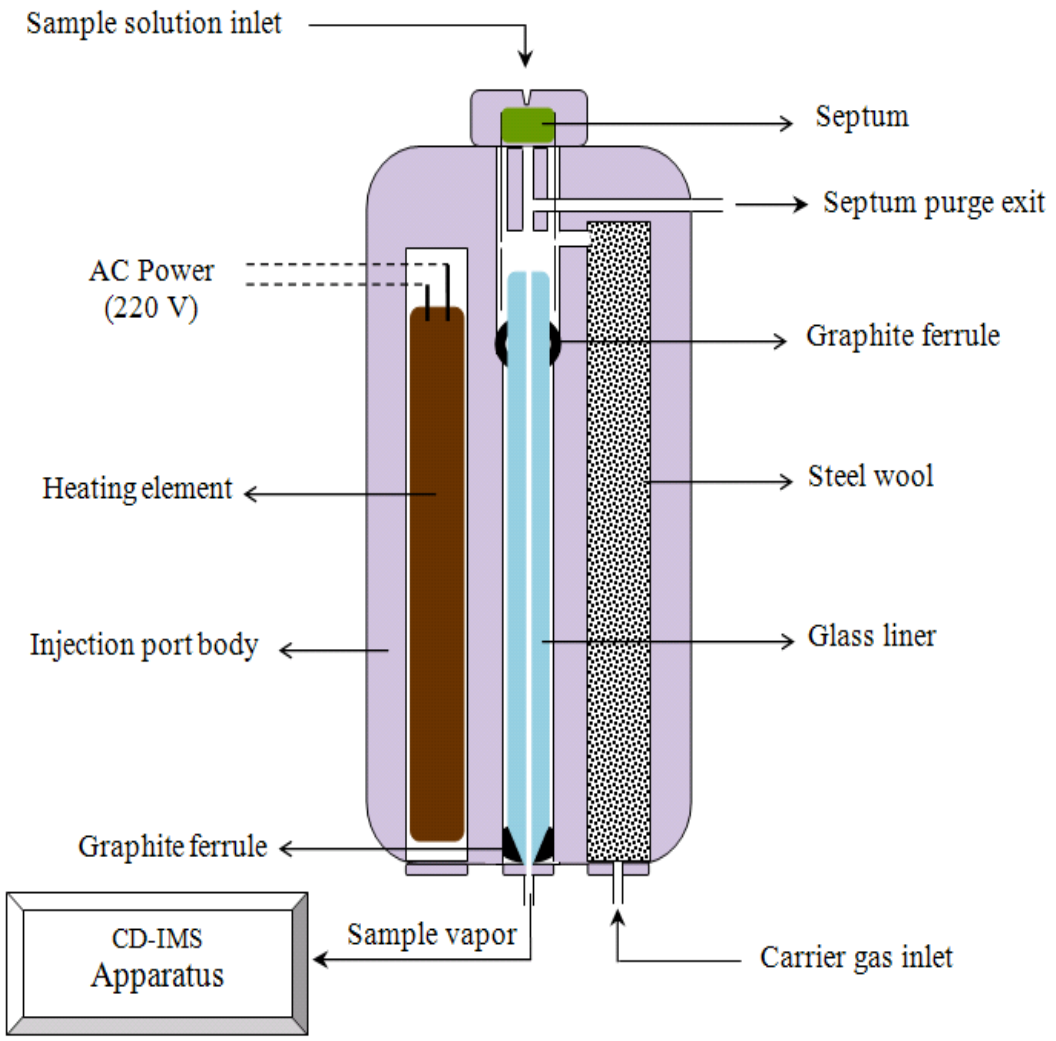
Quantitative Analysis



Sample Introduction System

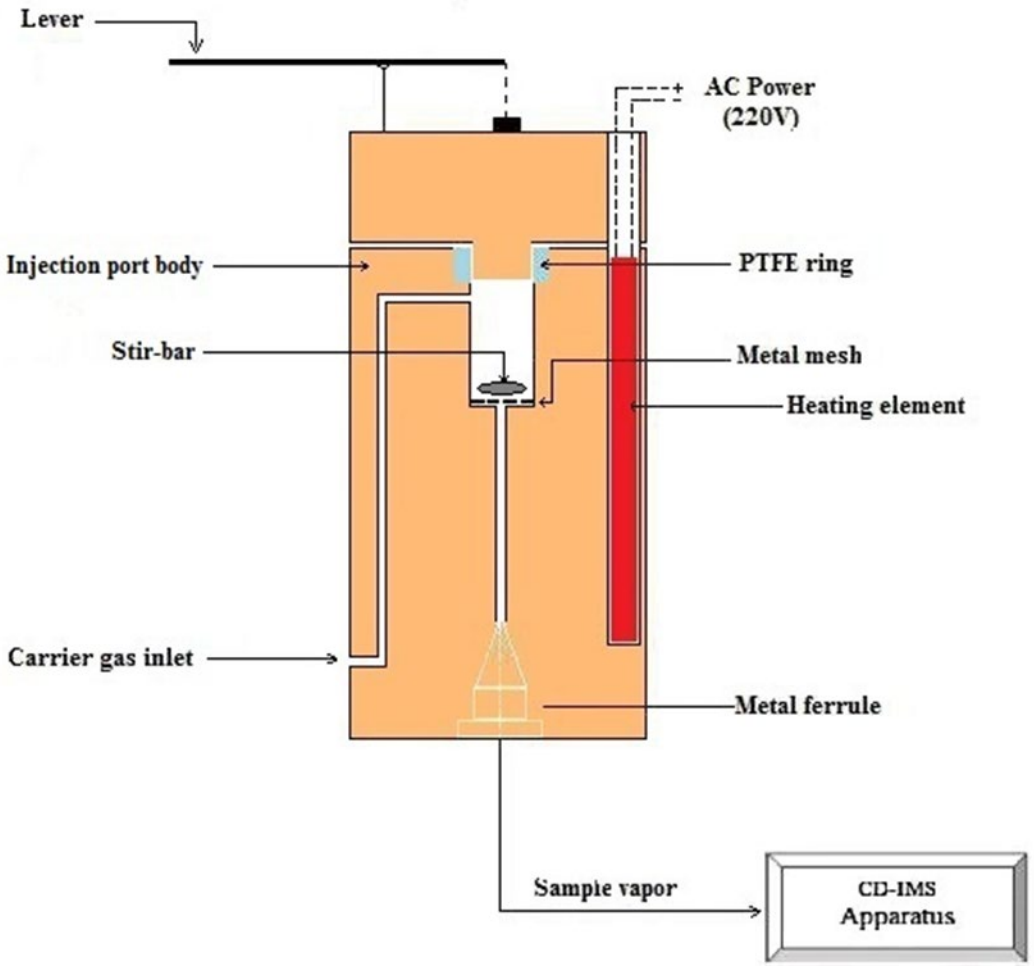


Sample Introduction System



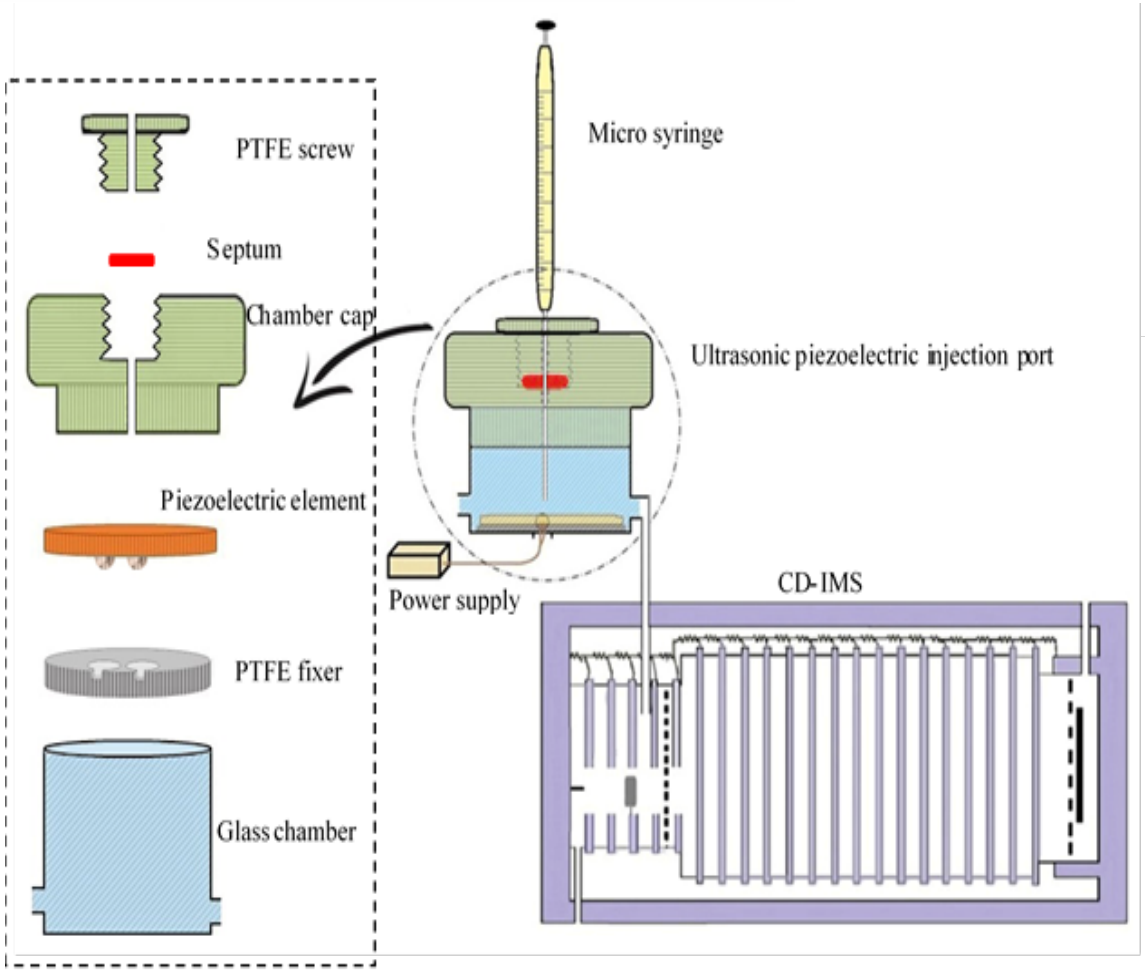
M.T. Jafari , F. Riahi, J. Chromatogr. A, 1343 (2014) 63–68.

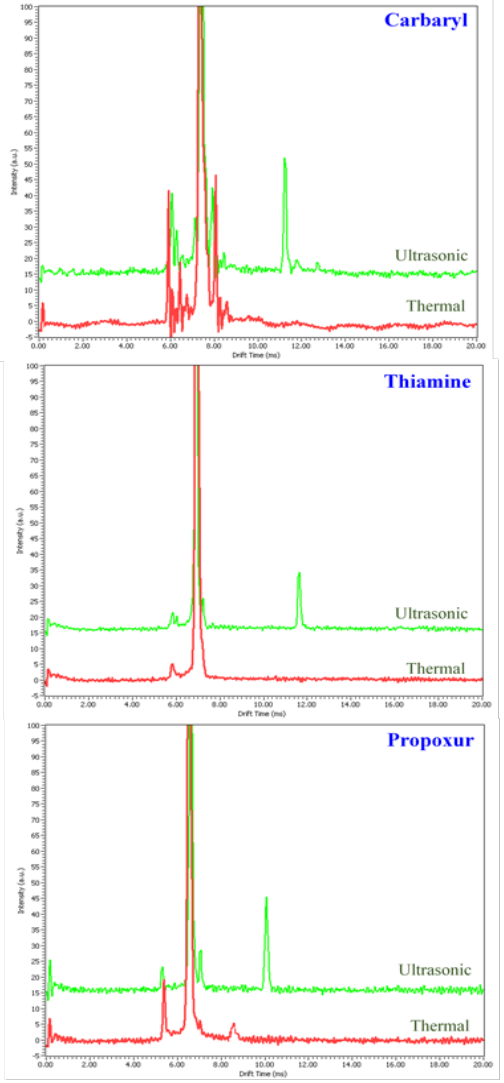
Sample Introduction System



M.T. Jafari , M.R. Rezayat, M. Mossaddegh, Talanta 178 (2018) 369–376.

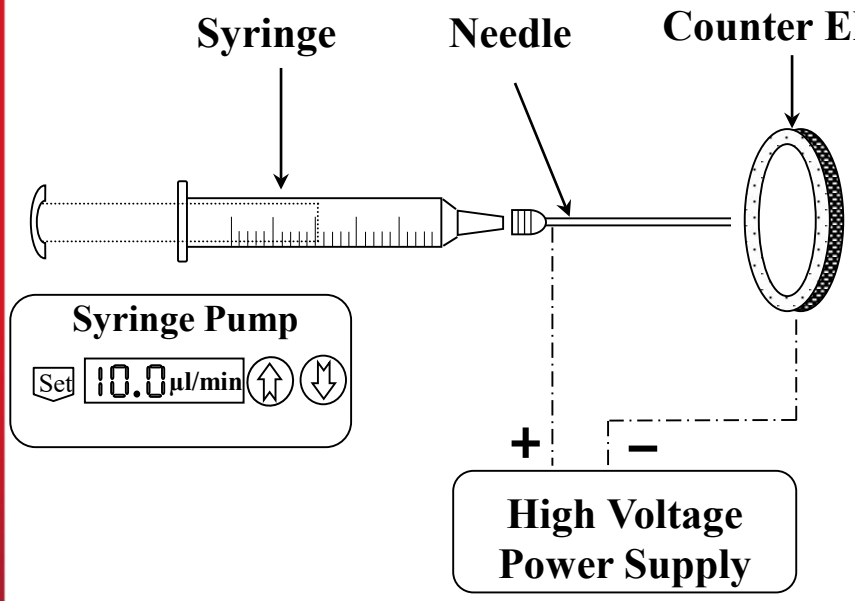
Sample Introduction System

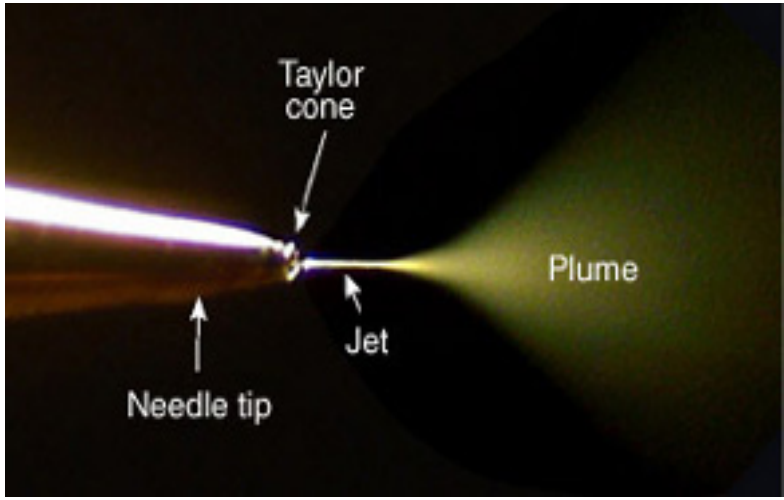


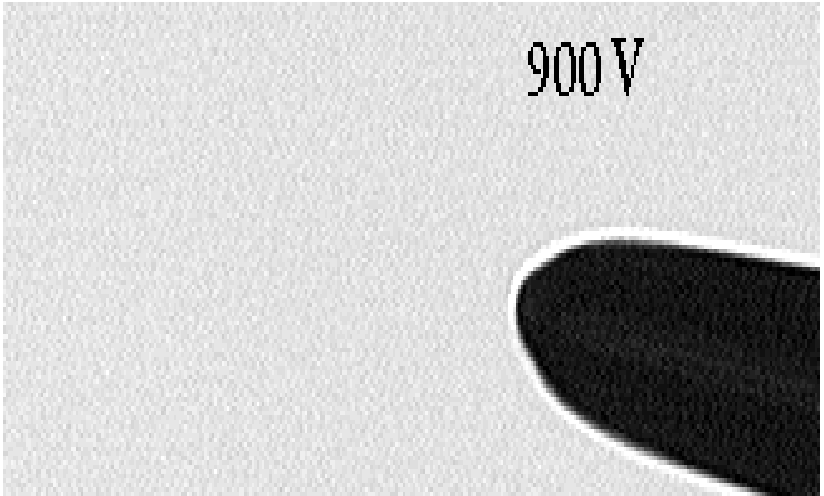


M.T. Jafari , S. Ramazani, Anal. Chim. Acta, 1038 (2018) 79–86.

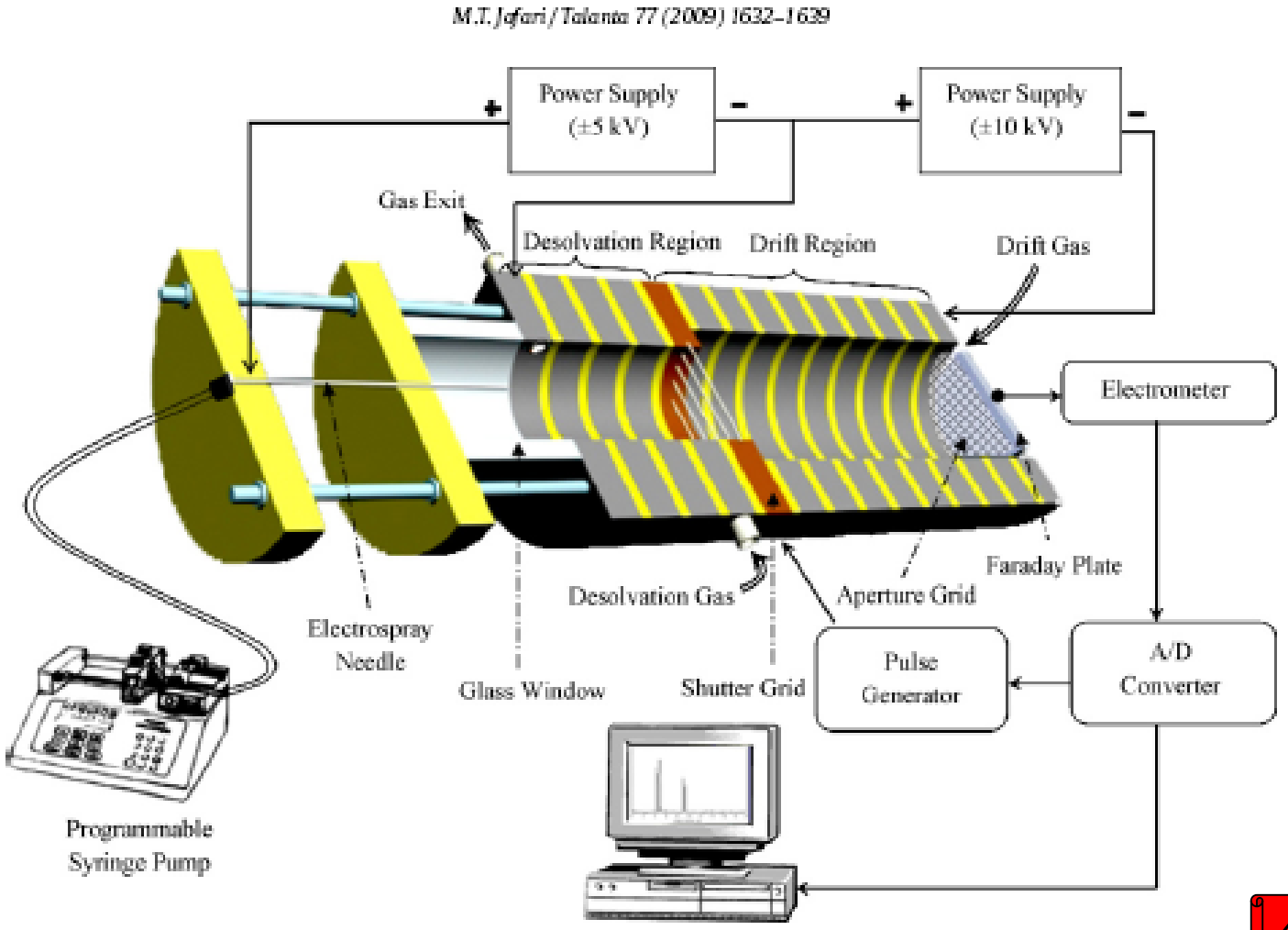
What is Electrospray?



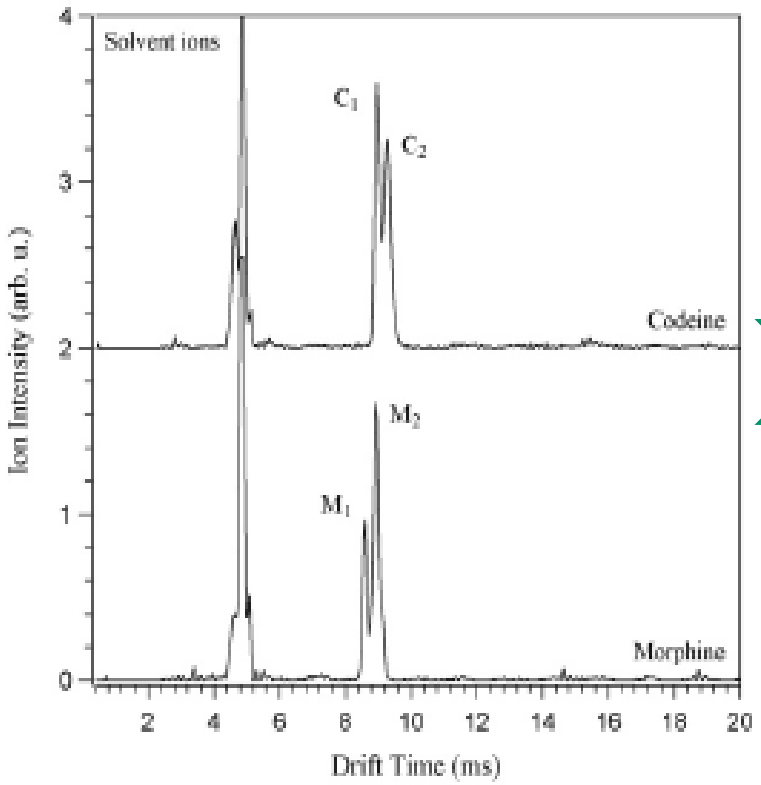


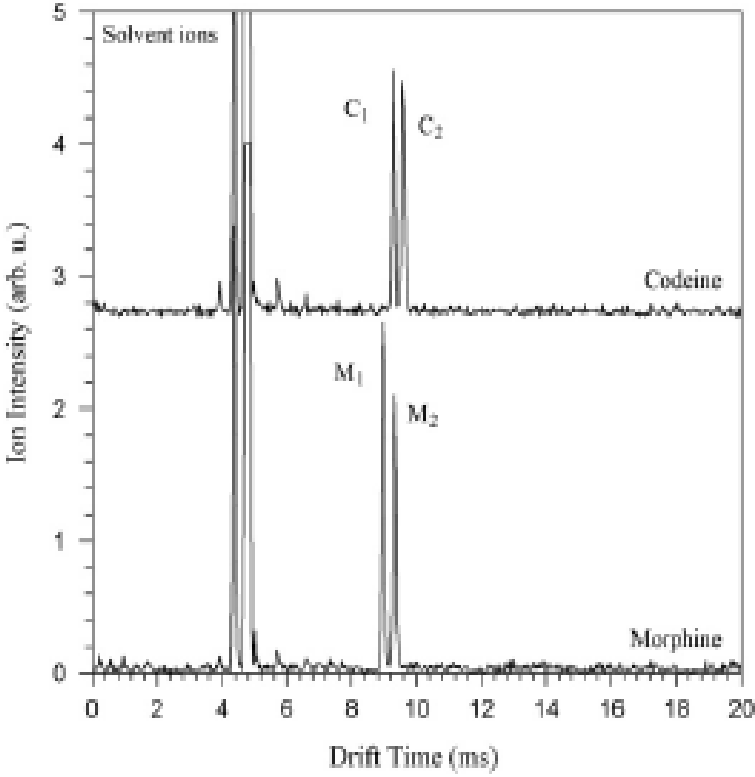


Improved Design for ESI–IMS

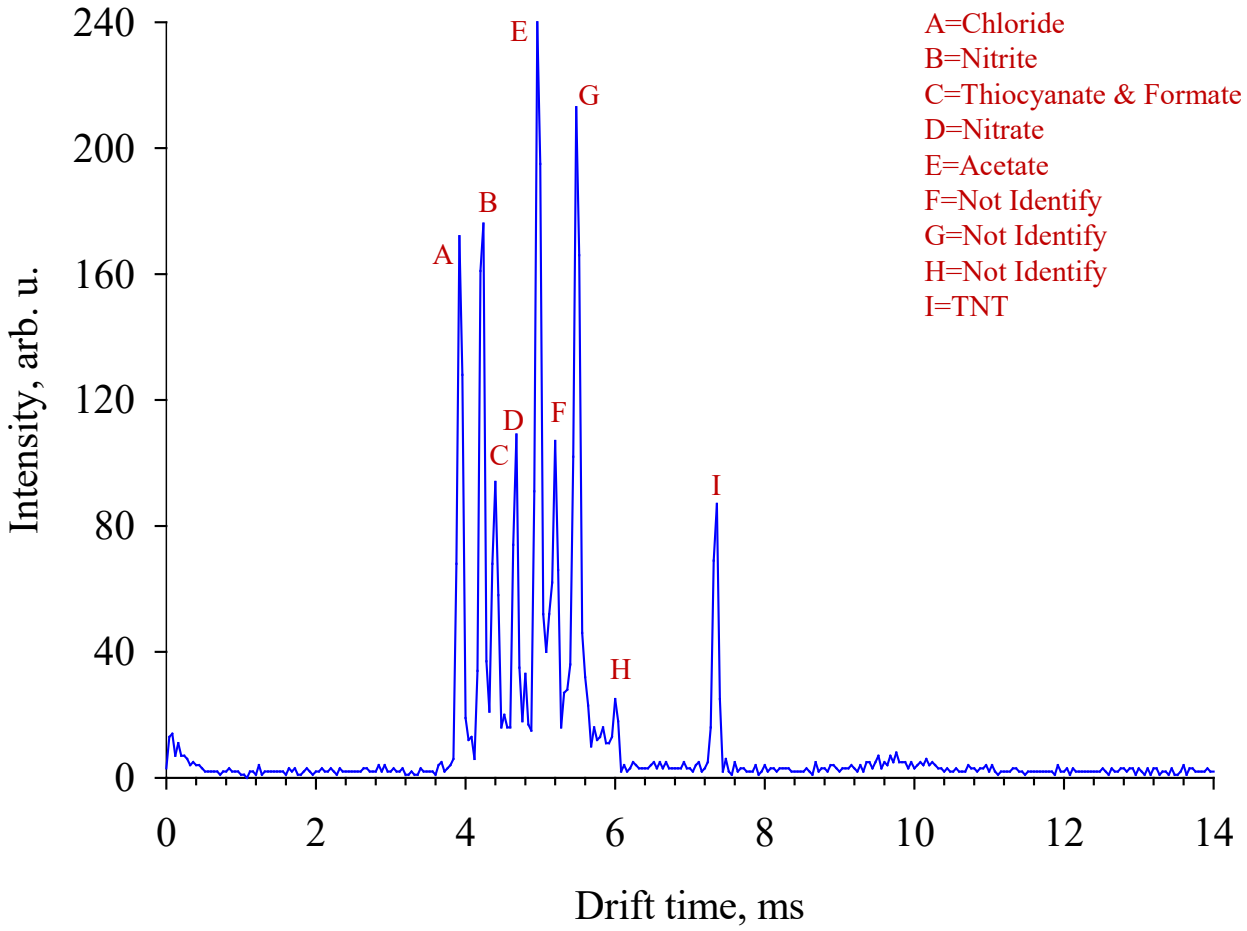


Improved Design for ESI–IMS

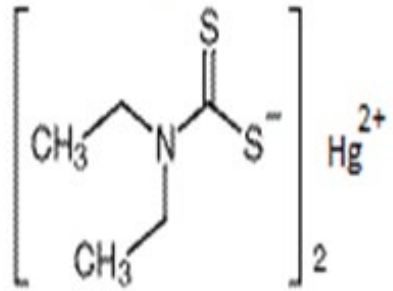


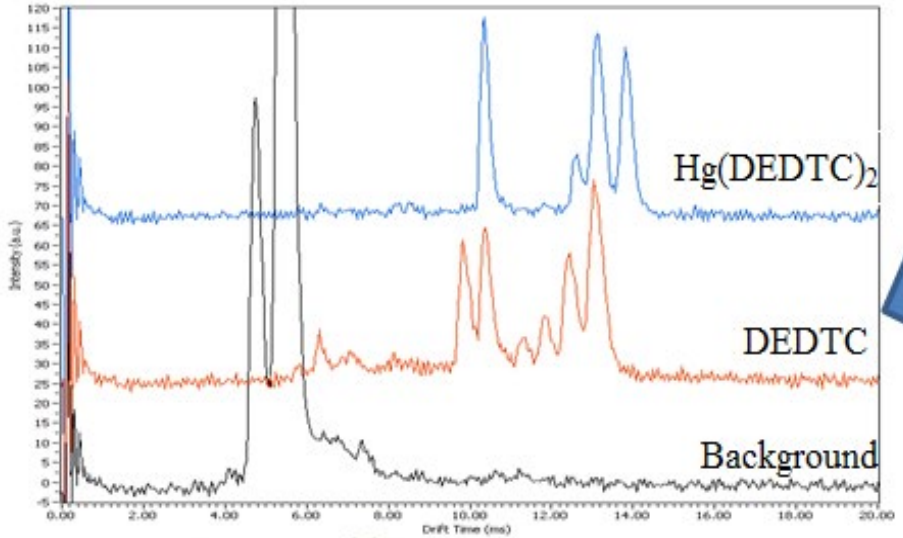


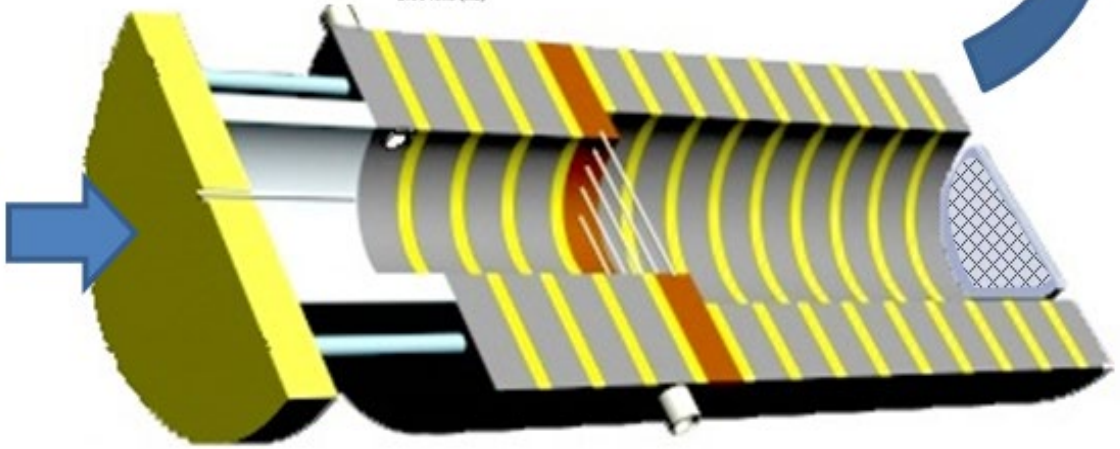
Direct Analysis of Salivary Thiocyanate



Metals Analysis Using CD-IMS

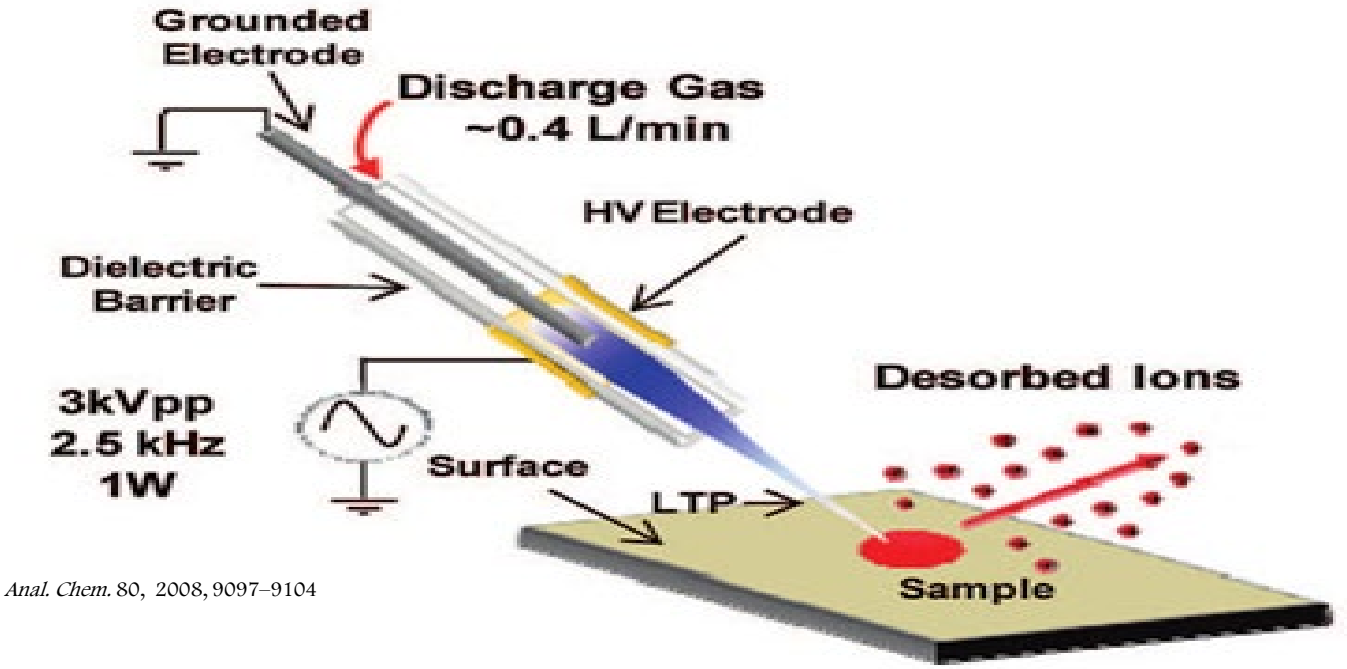






Diethyldithiocarbamate

Low Temperature Plasma (LTP)



Anal. Chem. 80, 2008, 9097–9104

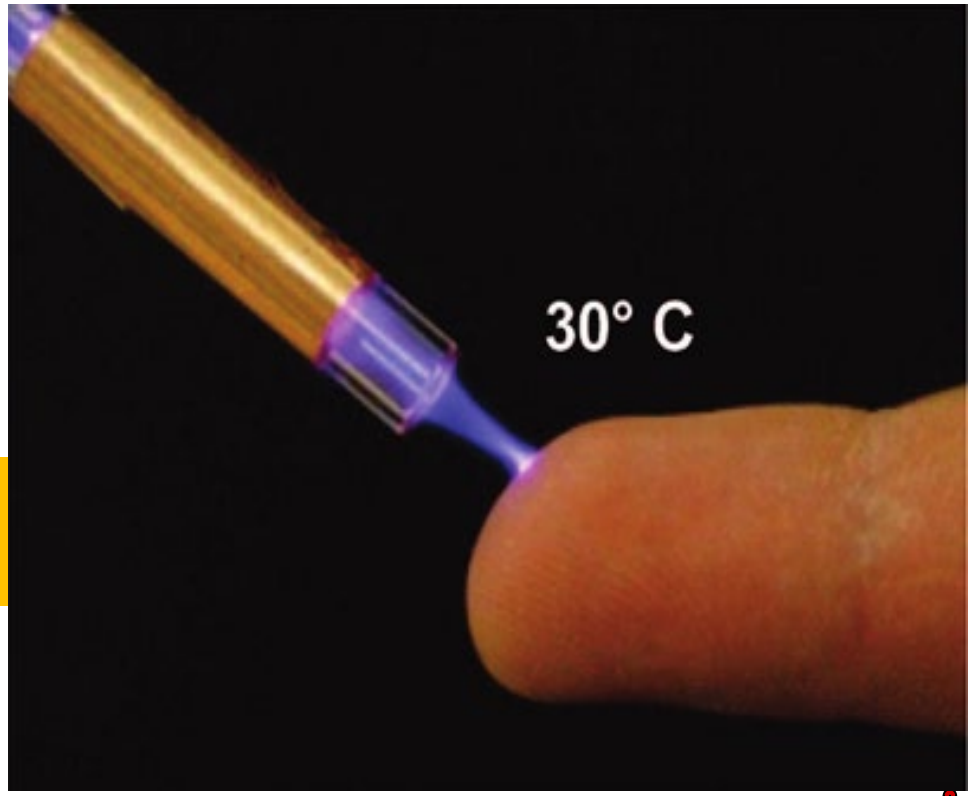
- electronic energy transfer, metastable gas atom, electron and ion impacts
- proton transfer between the reactant ions and evaporated molecules
- photoionization using ultraviolet light produced in the plasma

Low Temperature Plasma (LTP)

In LTP ionization, various discharge gases, such as helium, argon, nitrogen, and air, can be passed through the glass tube to facilitate the discharge and to transport analyte ions.

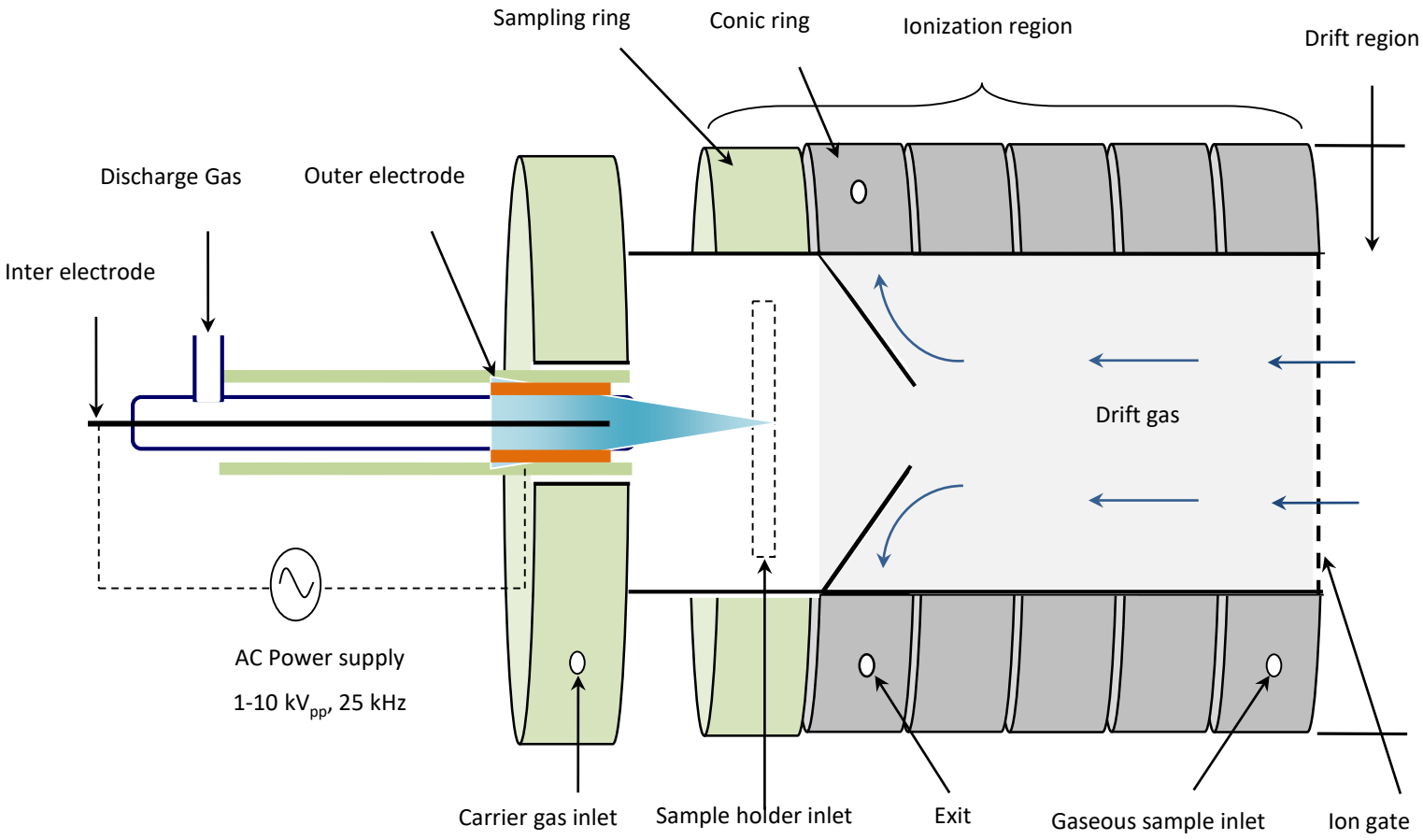
– no heating
– no electric shock

direct analysis of chemicals
even on a human finger



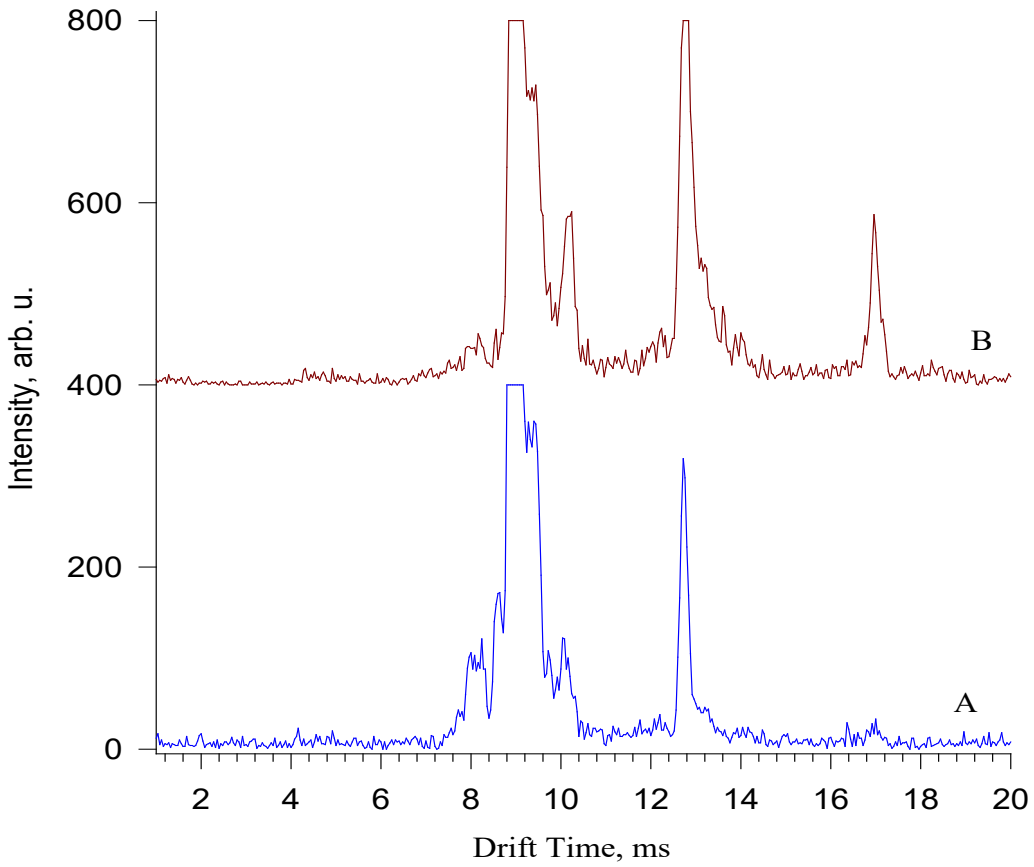
Anal. Chem. 80, 2008, 9097–9104

LTP–IMS



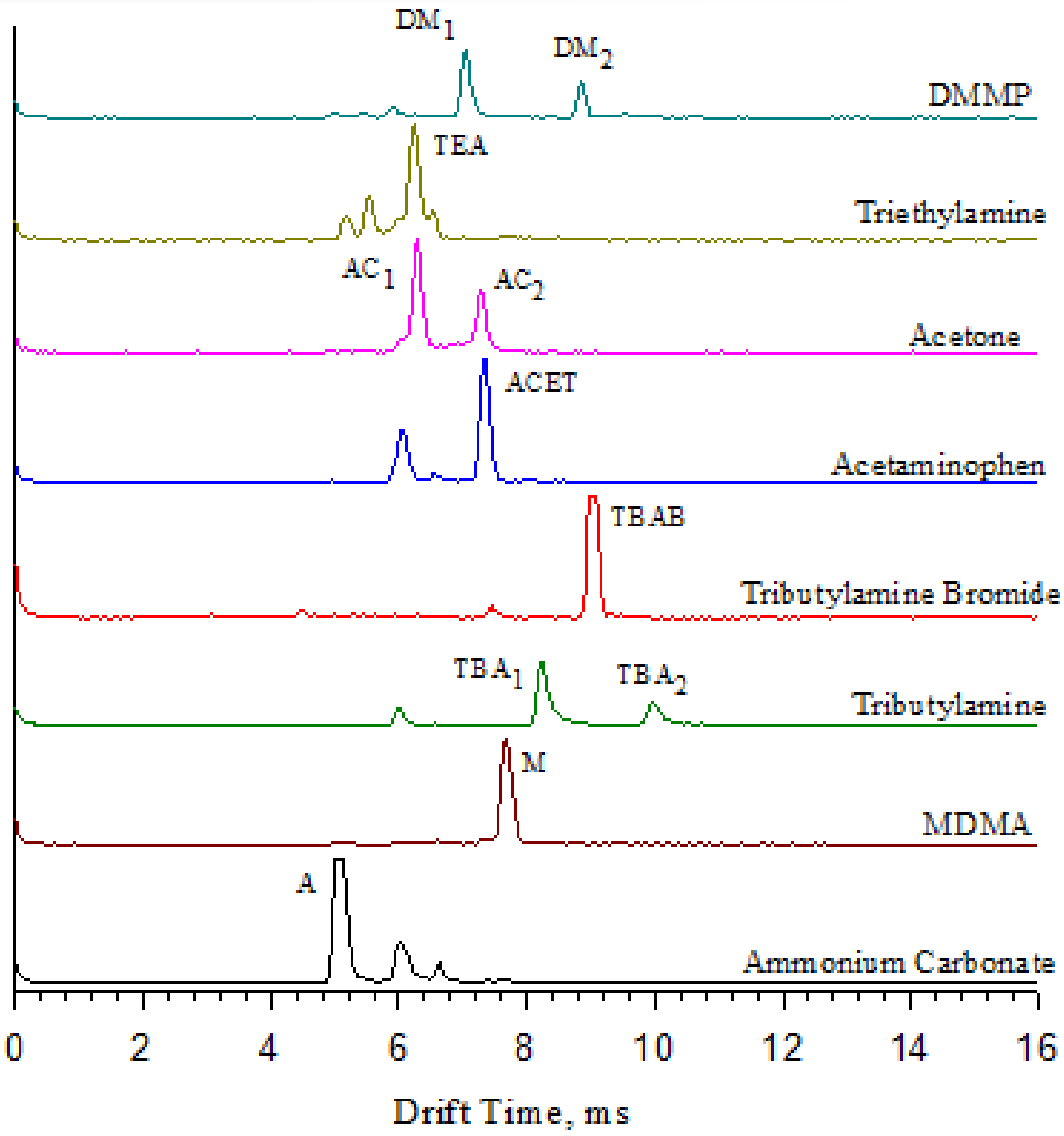
These reactant ions ionize the gaseous samples directly and liquids or solids after evaporation by plasma desorption.

TNT analysis by LTP–IMS

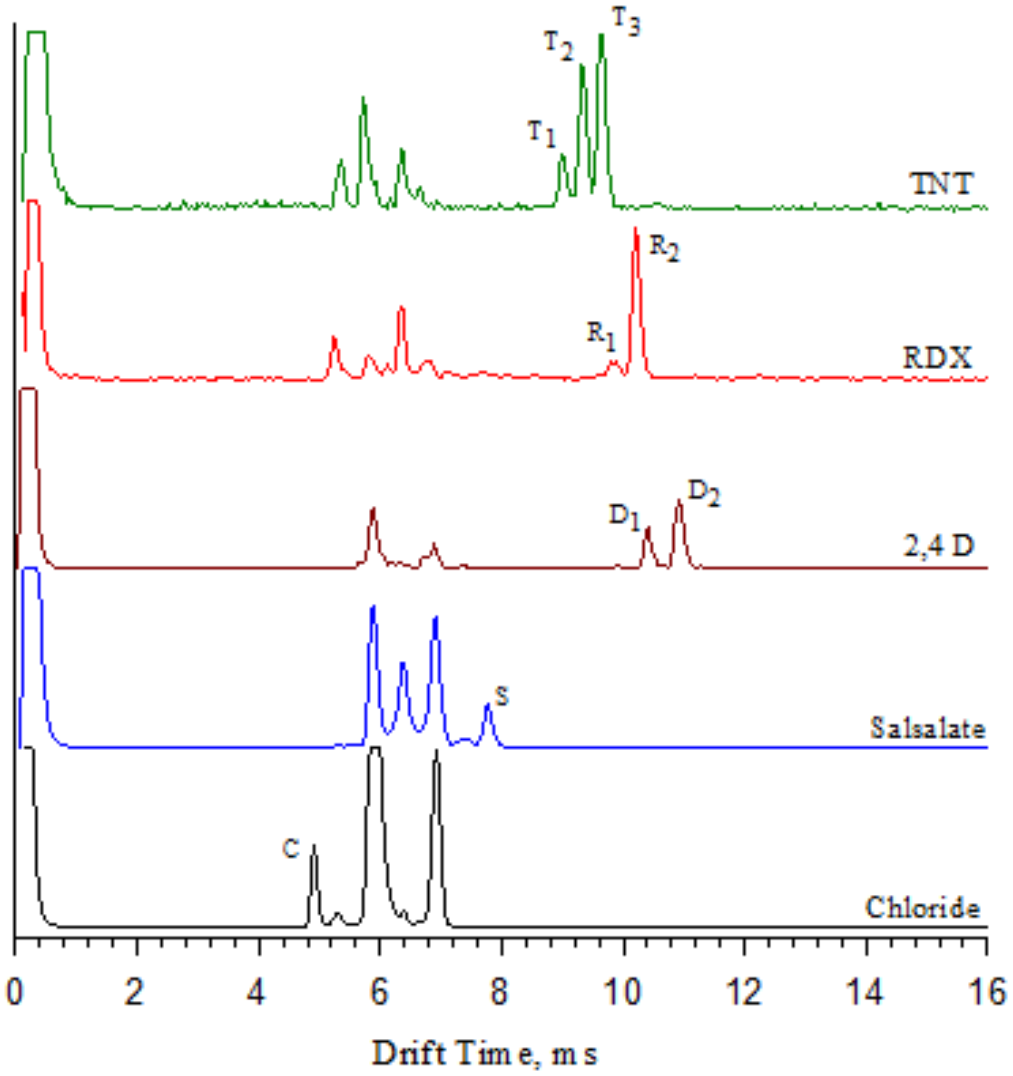


The ion mobility spectrum of TNT obtained by LTP-IMS in ambient temperature (~25 °C) A: without carrier gas and B: with carrier gas (Ar, 100 mL/min).

Characteristic ions (positive)

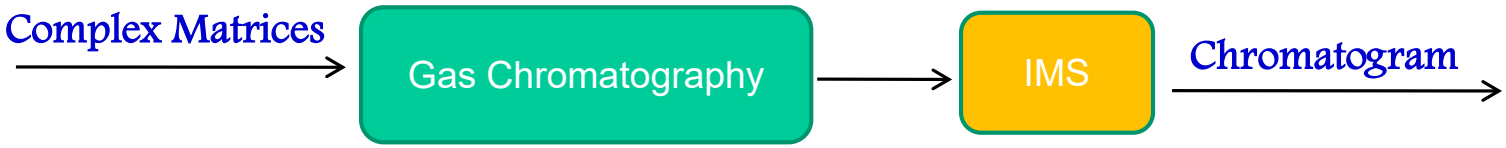


Characteristic ions (negative)



Hyphenated Techniques

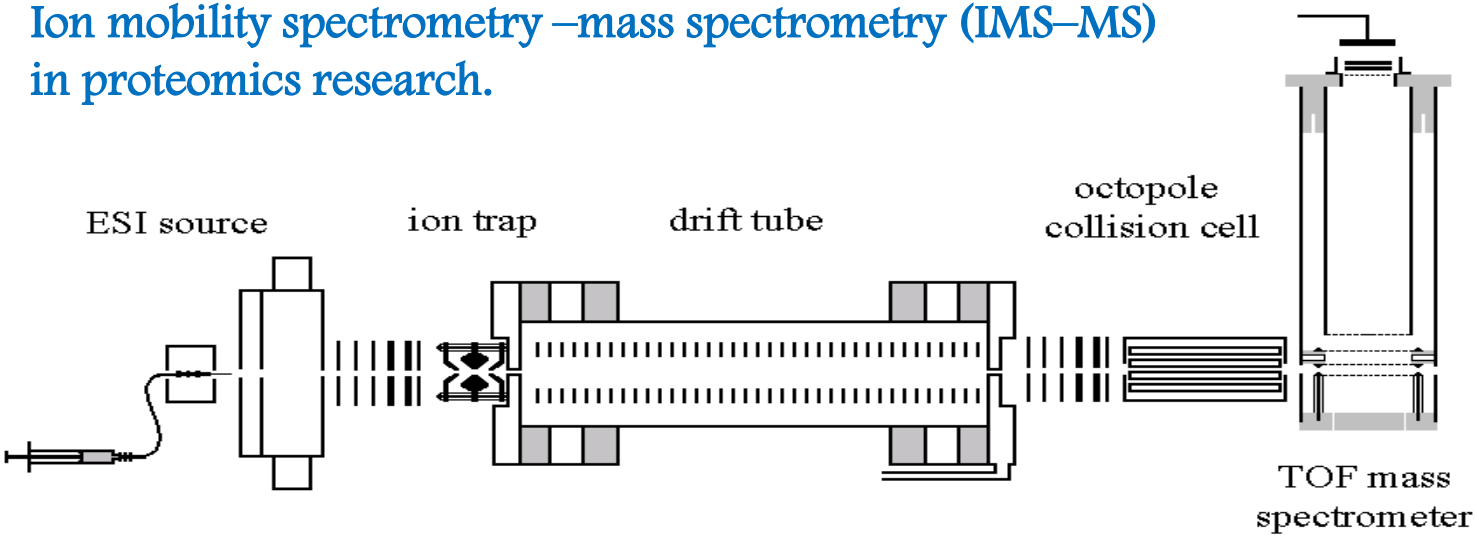
Gas chromatography–Ion mobility spectrometry (GC–IMS)



Liquid chromatography–Ion mobility spectrometry (LC–IMS)

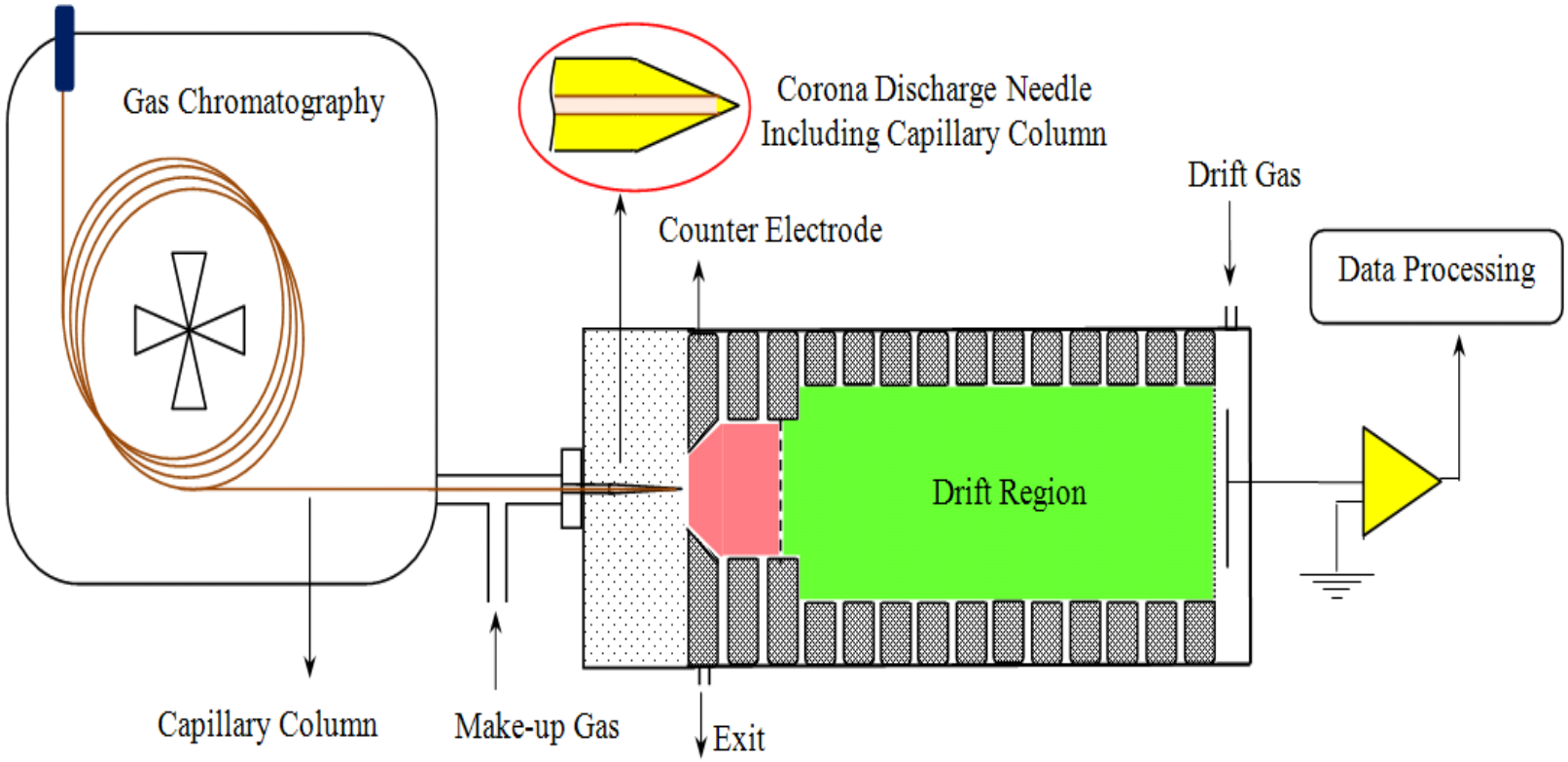
Super critical flouid chromatography–Ion mobility spectrometry (SFC–IMS)

Ion mobility spectrometry –mass spectrometry (IMS–MS) in proteomics research.



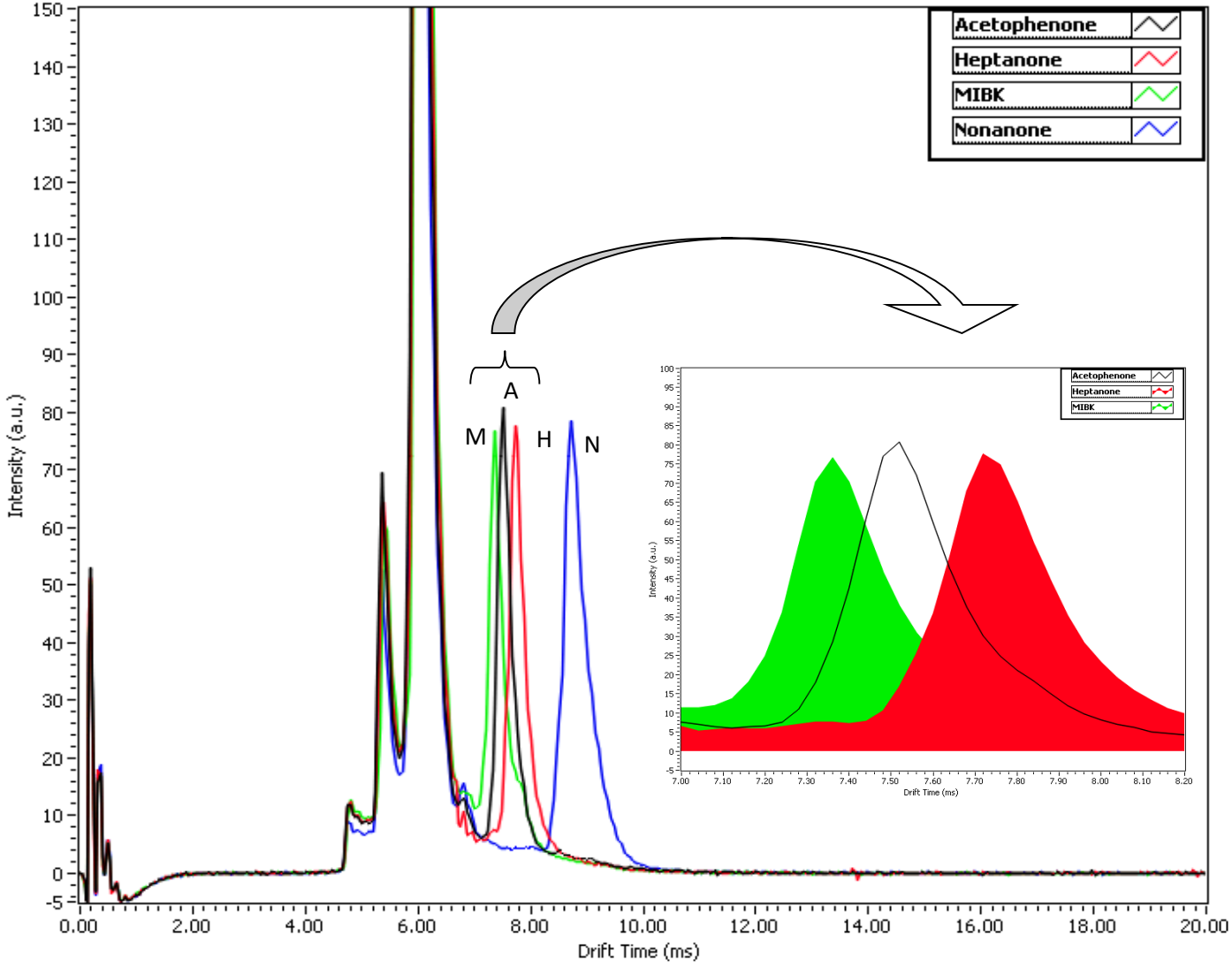
http://www.indiana.edu/~clemmer/Research/ion%20mobility/sequin/sequin.htm

GC–IMS

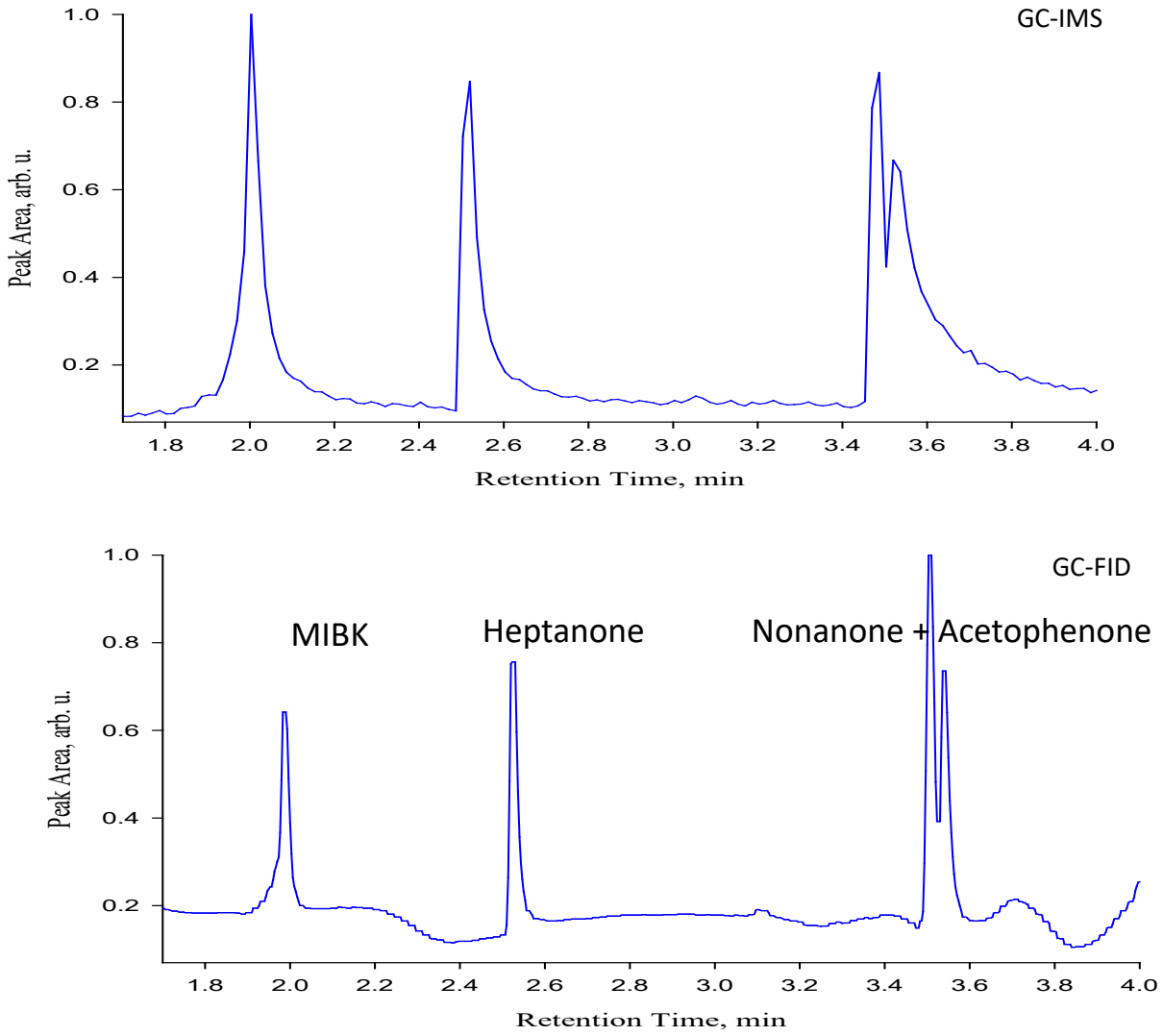

Gas Chromatography
Corona Discharge Needle
Including Capillary Column
Drift Gas
Counter Electrode
Data Processing
Drift Region
Capillary Column
Make-up Gas
Exit

GC–IMS

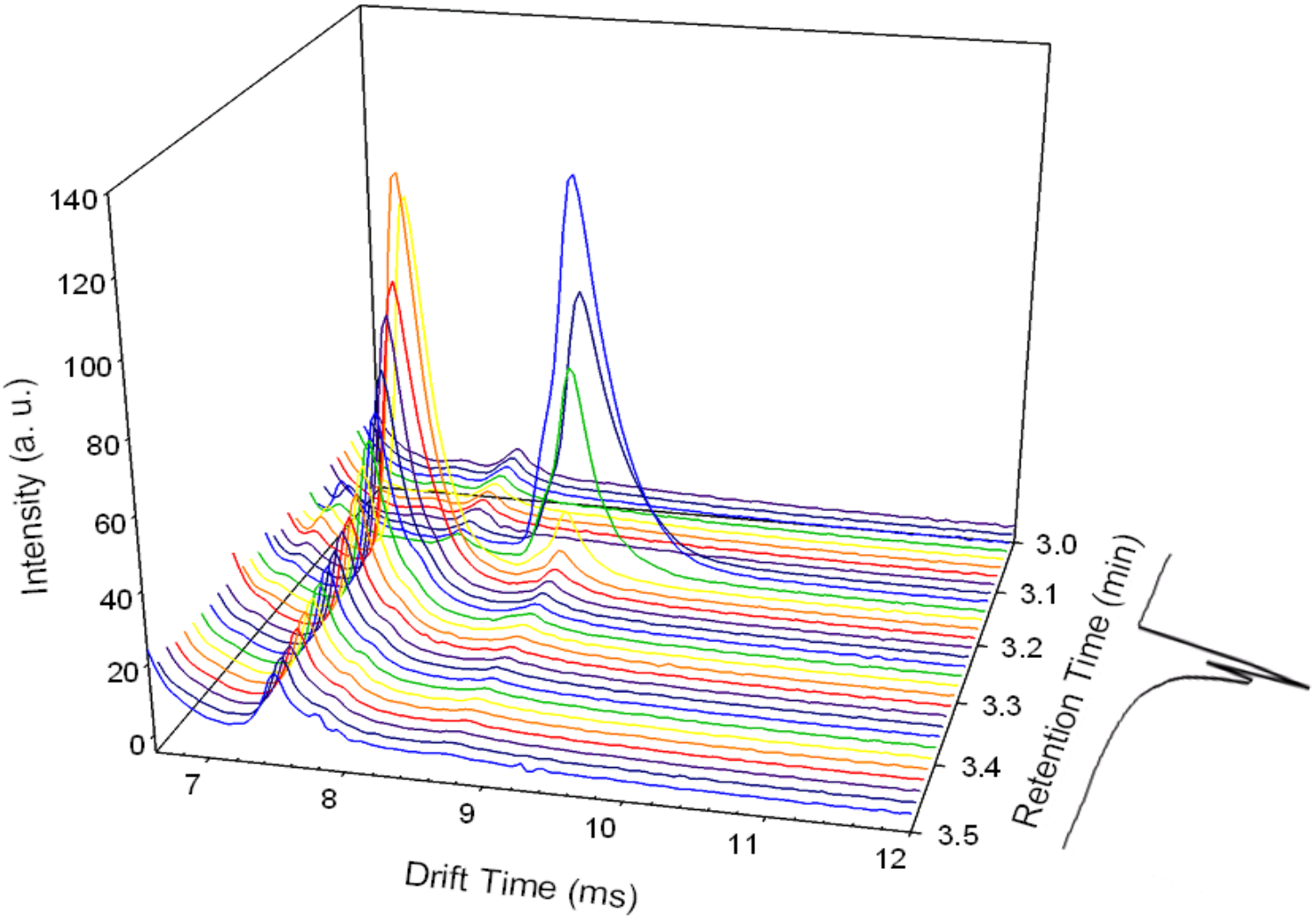
Ion Mobility Spectra



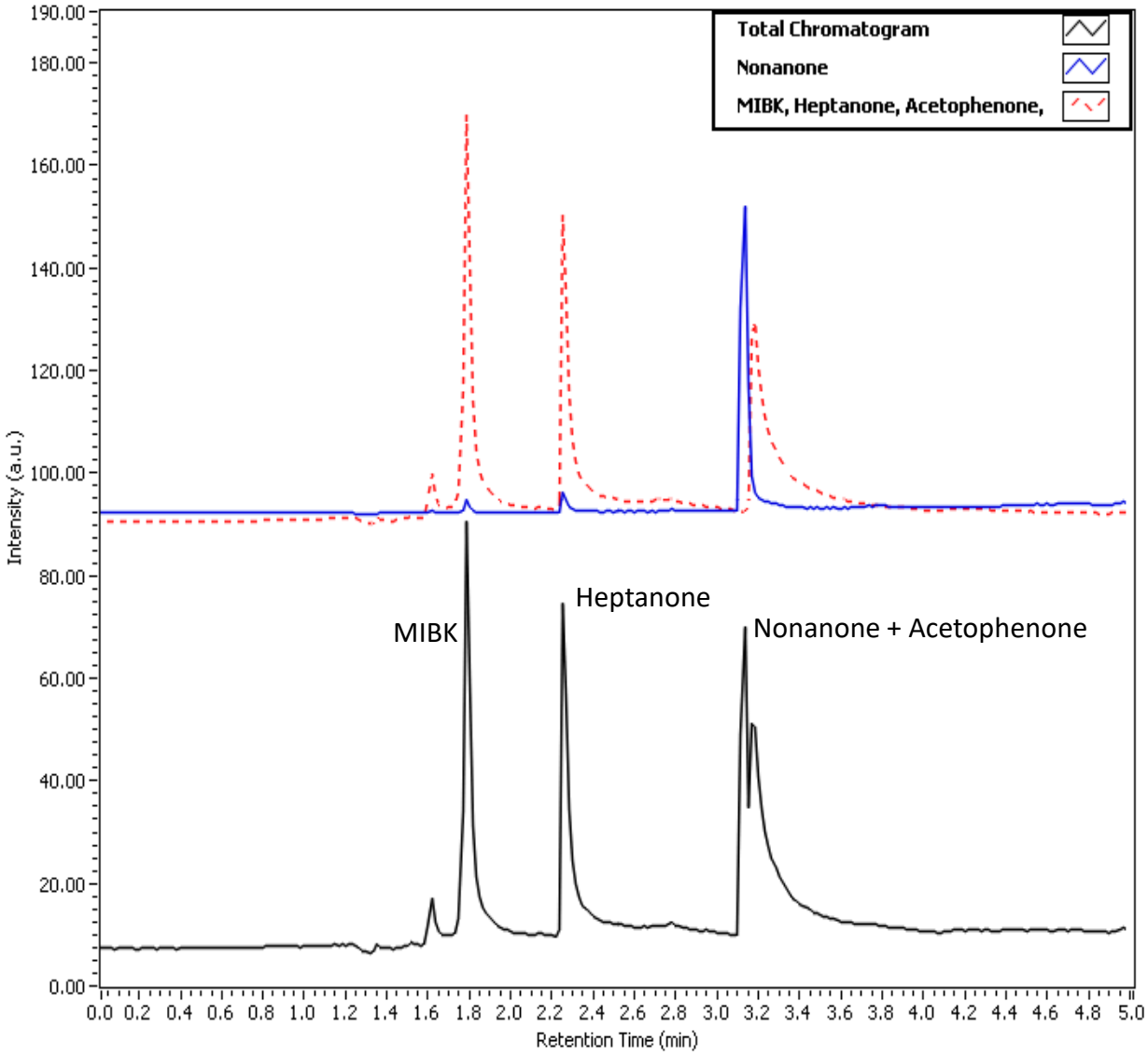
GC–IMS Chromatogram



3–D Plot of GC–IMS Response



Capability of GC–IMS



Combined extraction systems

Solid phase extraction (SPE) with CD-IMS

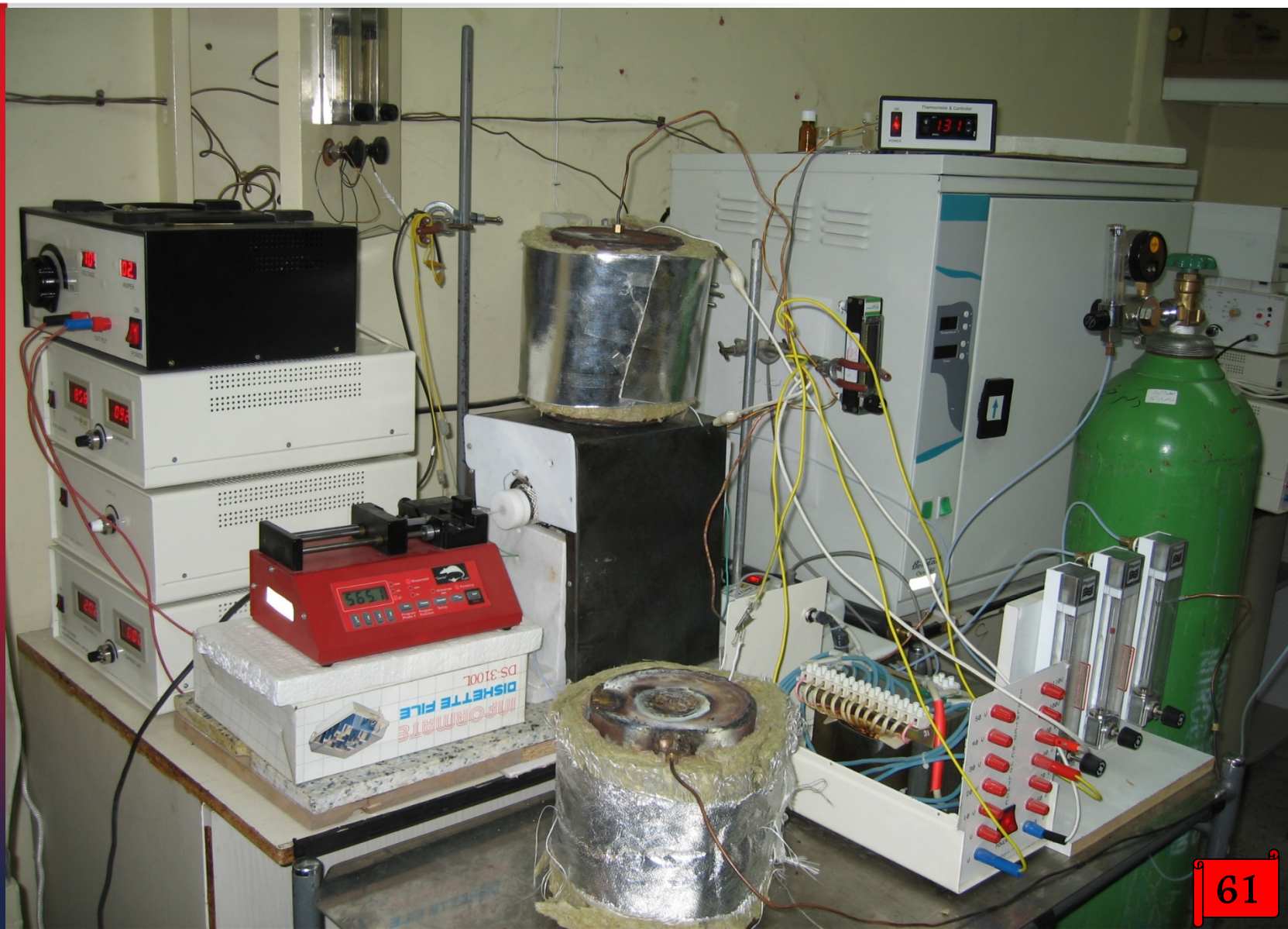
Microextraction in packed syringe (MEPS) with ESI-IMS

Molecular imprinted polymer (MIP) separation with CD-IMS

Hollow fiber-based liquid-liquid-liquid microextraction with ESI-IMS, CD-IMS, and GC-IMS

Dispersive liquid–liquid microextraction with ESI-IMS, CD-IMS, and GC-IMS

IMS (Prototype-1)



IMS (Prototype-2)

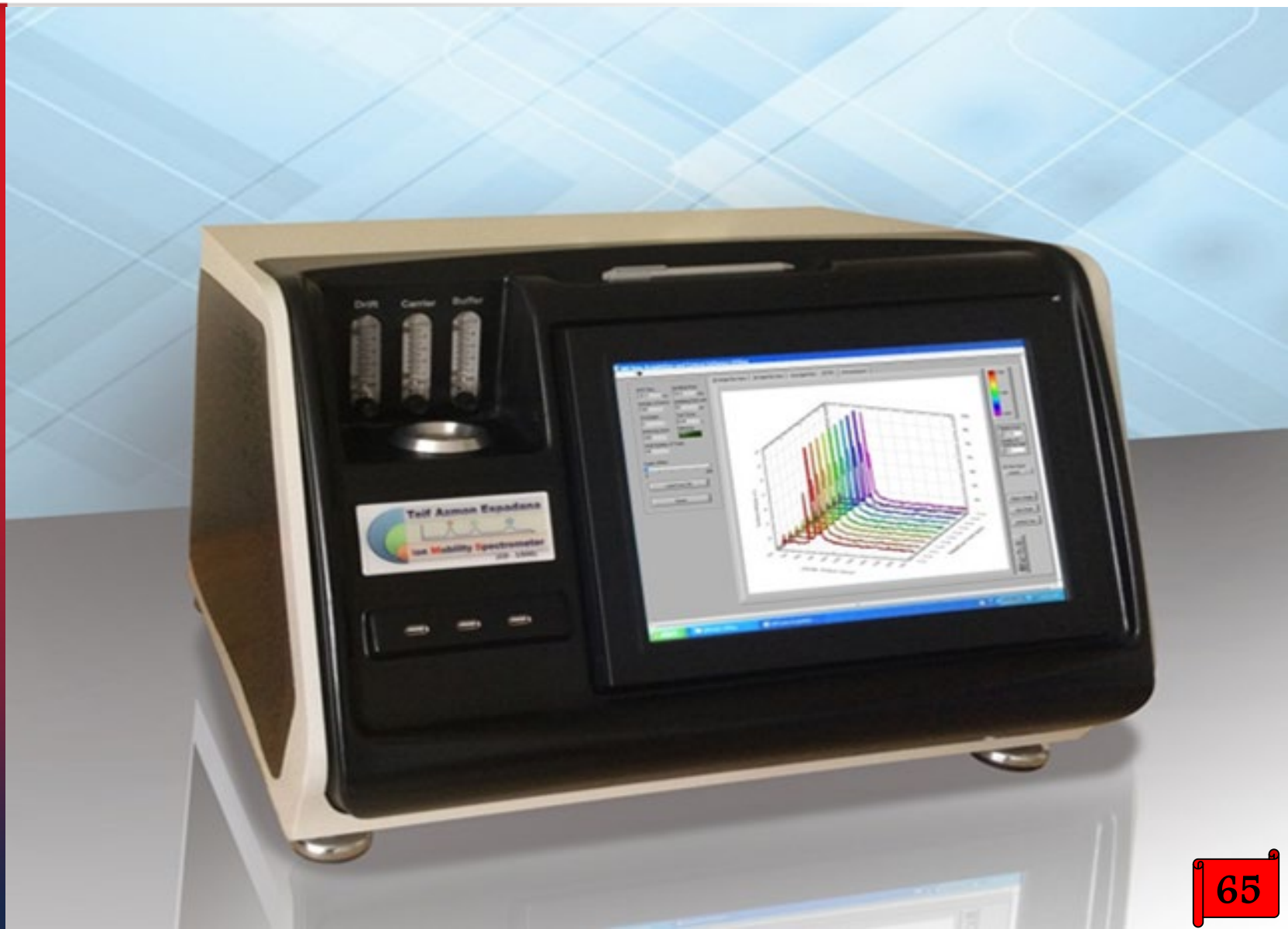
IMS (CD-1300)


Ion Mobility Spectrometer
CD-1300
IMS Operation Mode
Positive
Negative

IMS (CD-1400)


Drift
Carrier
Buffer
Teif Azmon Espadana
Ion Mobility Spectrometer
(CD - 1400)
Drift Voltage (kV)
7.00
Ionization Voltage (kV)
2.00
Pulse Width (µs)
070
Pulse Voltage (V)
150
Cell Temperature (°C)
182.9
Operation Mode
+
-
Injection Temperature (°C)
151.9

IMS (CD-1500)



Development process

Certificate

ریاست جمهوری
معاونت علمی و فناوری
ستاد ویژه توسعه فناوری نانو

واحد ارزیابی تجهیزات

گواهینامه ارتباط با نانو

شماره گواهینامه: ۹۶/ک ت/۲۶۱۷

بر اساس این گواهینامه

دستگاه

طیف‌سنج تحرک یونی با مدل‌های

"CD-1400 , CD-1500"

شرکت

طیف آزمون اسپادانا

با شناسه ملی ۱۰۴۰۰۴۳۹۳۱۰۵

طبق استاندارد ISO/TS 18110 در حوزه فناوری نانو قرار می گیرد.

استفاده از این گواهینامه تنها برای این محصول معتبراست و سایر محصولات شرکت را شامل نمی‌شود.

تاریخ صدور	تاریخ اعتبار
۱ آذر ۱۳۹۹	۳۰ آبان ۱۴۰۲

اعتبار این گواهینامه پس از ارزیابی مجدد قابل تمدید خواهد بود.

سعید سرکار
دبیر ستاد

واحد ارزیابی تجهیزات و ماشین آلات صنعتی
تهران، خیابان ستارخان، خیابان شهید حبیب الله، خیابان شهید متولیان، پلاک ۹، ستاد ویژه توسعه فناوری نانو
تلفن: ۰۲۱-۶۳۱۰۰
www.nanoinst.ir

Certificate

جمهوری اسلامی ایران
وزارت علوم تحقیقات و فناوری

شهرک علمی و تحقیقاتی اصفهان

تاریخ: ۹۹/۰۲/۲۲
شماره: ۵۸۰/ص/۹۹

مجوز واحد فناوری

به منظور توسعه اقتصاد دانش بنیان، به

شرکت طیف آزمون اسپادانا

دارای شناسه ملی ۱۴۰۰۴۳۹۳۱۰۵، به استناد مجوز استقرار شماره ۲۳۹۶ مورخ ۹۵/۵/۲۰ اجازه داده می شود در زمینه تخصصی

اسپکترومتر تحرک یونی

به عنوان واحد فناوری در شهرک علمی و تحقیقاتی اصفهان فعالیت نماید.

جعفر قیصری
رئیس شهرک علمی و تحقیقاتی اصفهان

اعتبار این مجوز از تاریخ ۹۹/۱/۱ تا تاریخ ۹۹/۱۲/۲۹ می باشد.
این مجوز بدون مهر و لوگرام و مهر برجسته فاقد اعتبار است.
به مندرجات ظهر برگ توجه شود.

اصفهان، بلوار دانشگاه صنعتی اصفهان، شهرک علمی و تحقیقاتی اصفهان، کد پستی: ۸۴۱۵۶۸۳۱۱۱ | صندوق پستی: ۶۶۶-۸۴۱۵۵ | تلفن: ۳۳۸۶۵۴۵۵-۰۳۱ | نمابر: ۳۳۸۶۲۳۵۵-۰۳۱ | www.istt.ir

IMS Users

	Domestic Users
1	Isfahan University of Technology
2	Ministry of Defence
3	University of Kashan
4	University of Tehran
5	Shahid Bahonar University of Kerman
6	Materials and Energy Research Center
7	Shahid Chamran University of Ahvaz
8	Kharazmi University
9	University of Isfahan
10	Alzahra University
11	Imam Hossein University
12	Shahroud University of Technology
13	Shahid Beheshti University
14	Yasouj University
15	Urmia University of Medical Sciences
16	Gonbad Kavous University
17	Zanjan University of Medical Sciences
	Abroad Users
	Cuban Center for Advanced Studies (CEA), Cuba

Current Projects

- Commercial Model of GC-IMS
- Commercial Model of ESI-IMS
- Design and manufacturing of FAIMS
- Design and manufacturing of TWIMS

Special Thanks

- Prof. Taghi Khayamian

(He never gave me fish, but taught me to fish!)

- My colleagues especially in Analytical Chemistry Group
- My MSc and PhD students
- Isfahan University of Technology (For financial support)

and finally all my colleagues at:

Teif Azmon Espdana

Thanks