Mass Spectrometry, Chromatography, Chemistry ….what is the purpose?

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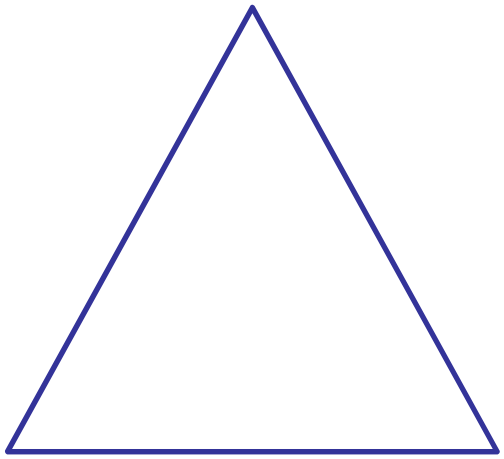
"Science without religion is lame, religion without science is blind "
(Albert Einstein)

Structure of lecture

- Introduction
- Historical perspective
- Personal research experience, with emphasis on recent years
- Vision for the Department

Understanding the exponential growth in scientific knowledge

technology (facilities)

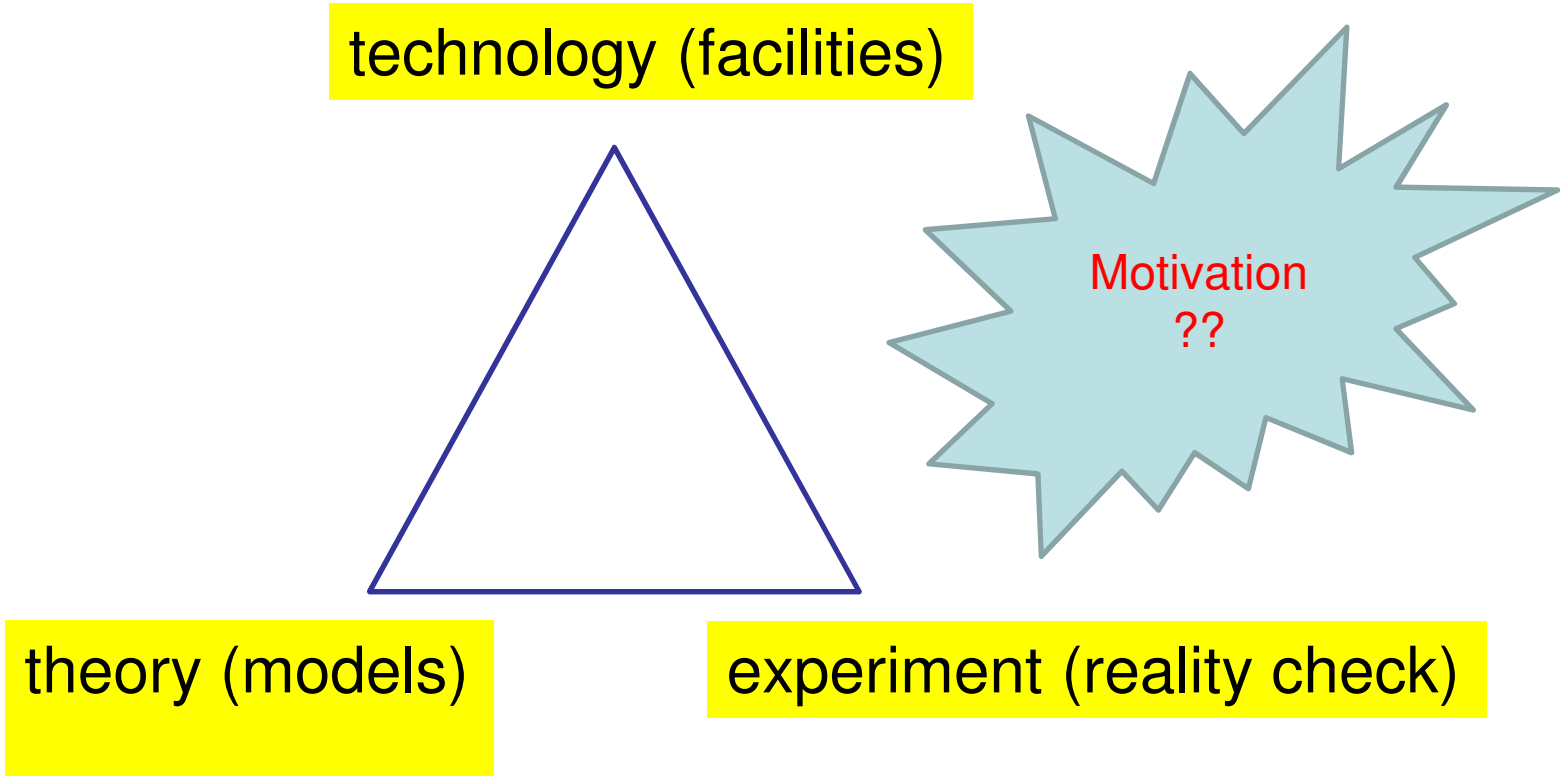


theory (models)

experiment (reality check)

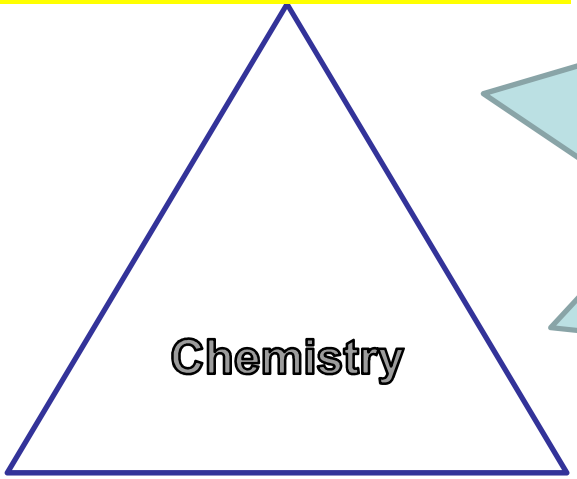
Older view: theory (models) ⇆ experiment (reality check)

Understanding the exponential growth in scientific knowledge



Exponential growth in the discipline: Chemistry

Analytical technology (facilities) “Toolbox”
MS, NMR, Xray Diff…
Computers



Motivation:
Curiosity/Aesthetics
Quality of life
Power/control

Chemical theory (models)

Application to real problems.
Experiment (reality check)

Chemistry – the central science

- The scientific discipline that bridges the mathematical, physical and biological sciences

  The non-living (inorganic) and living world can in principle be described in exact chemical terms considering atomic and molecular building blocks. In many instances we are still, however, quite far from such a detailed understanding.

Chemistry plays a critical role in most modern research programmes, including those of medicine, veterinary science and engineering

- The science that studies the composition, interaction, transformation of matter and the associated energy transformations

(internal combustion engines, digestion, photosynthesis, batteries, fuel cells, photoluminescence, oil-from-coal)

- The science that studies the properties and reactivity of matter by considering its atomic and molecular building blocks

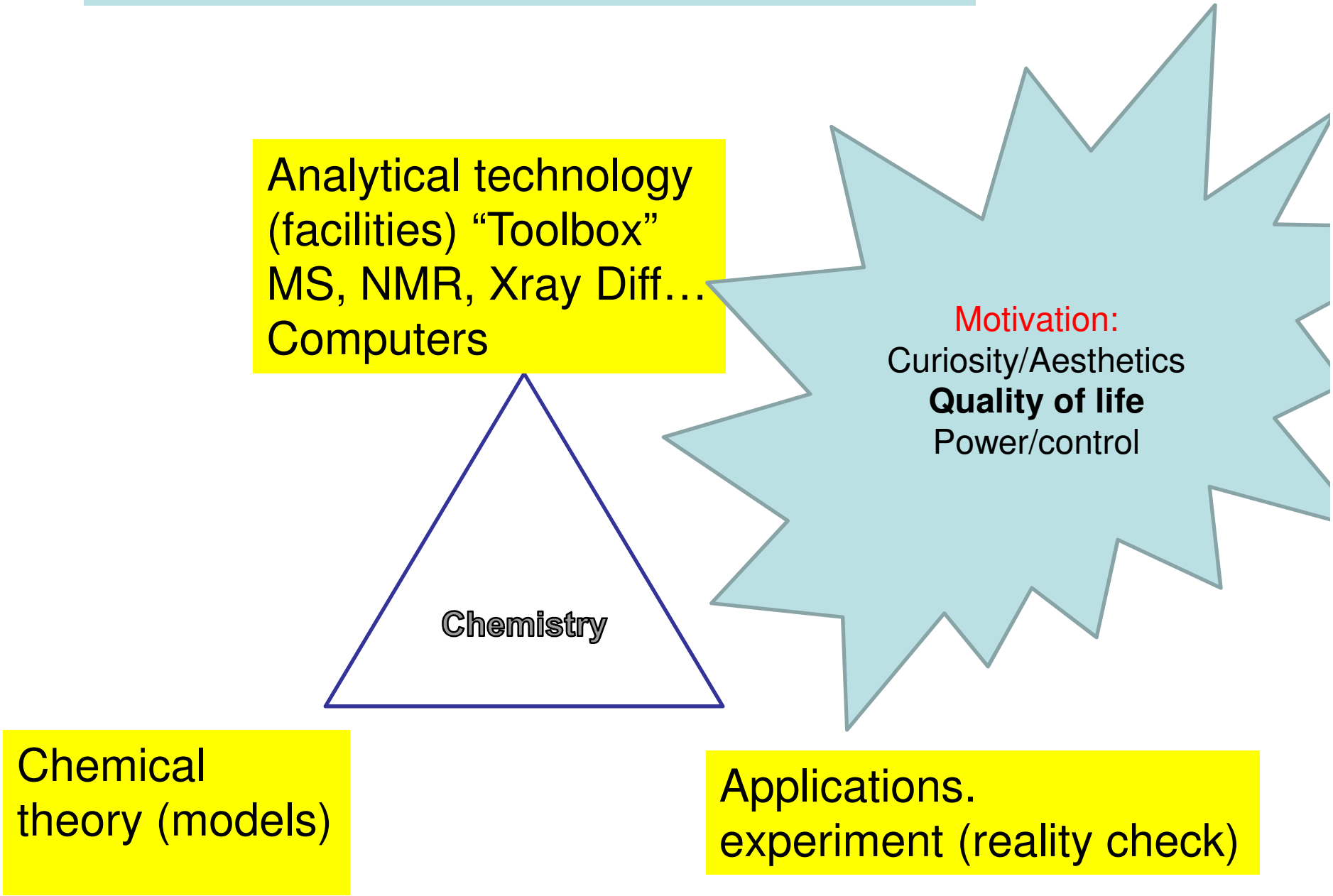
(bioprospecting, design of new drugs, MR and PET scans, diagnosis and treatment of cancer, design of new composite materials, photovoltaics, understanding the immune system, neurological activity)

Application: Revolutionary breakthroughs in Chemistry are required to address the major challenges of modern society.

Addressing poverty, improving the quality of life : "Sustainable Development"

- Reliable energy supply (also off-grid, transportable forms of energy)
- Environmental issues (especially considering global warming and carbon dioxide emission; dangerous pollutants like endocrine disrupters)
- Sustainable, safe food supply (GM foods, fertilizers, pest control and pesticide residues…)
- Health (stem cell research, antibiotics, AIDS, TB, Malaria, depression, Alzheimers, diabetes …)
- Clean water (sterilization, recycling, desalination ….)
- Safety and security (forensic chemistry in e.g. murder cases, detecting narcotics, explosives or other contraband)
- Education (- is the most powerful weapon to change the world (Nelson Mandela))

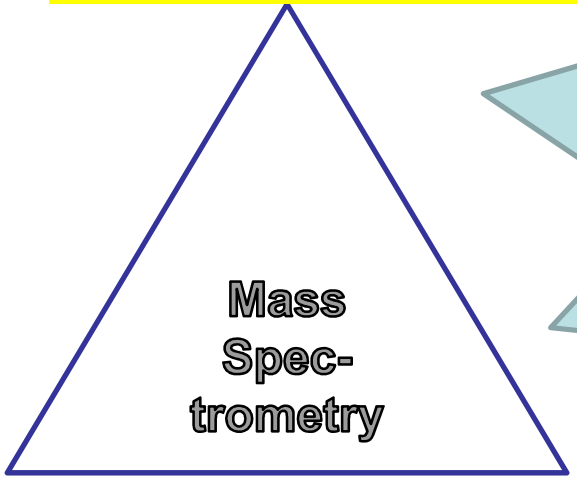
Exponential growth in the discipline: Chemistry



Exponential growth in sub-discipline: Mass Spectrometry

Electronics
Vacuum technology
Physics
Computers
Lasers
New devices

Motivation:
(i) Sustainable development
(ii) Expanding the technology toolbox ("senses") of chemistry



MS Equipment development

Sample Analysis
Analytical information
SERVICE to others

Structure of lecture

- Introduction
- Historical perspective (MS, Chrom.)
- Personal research experience, with emphasis on recent years
- Vision for the Department

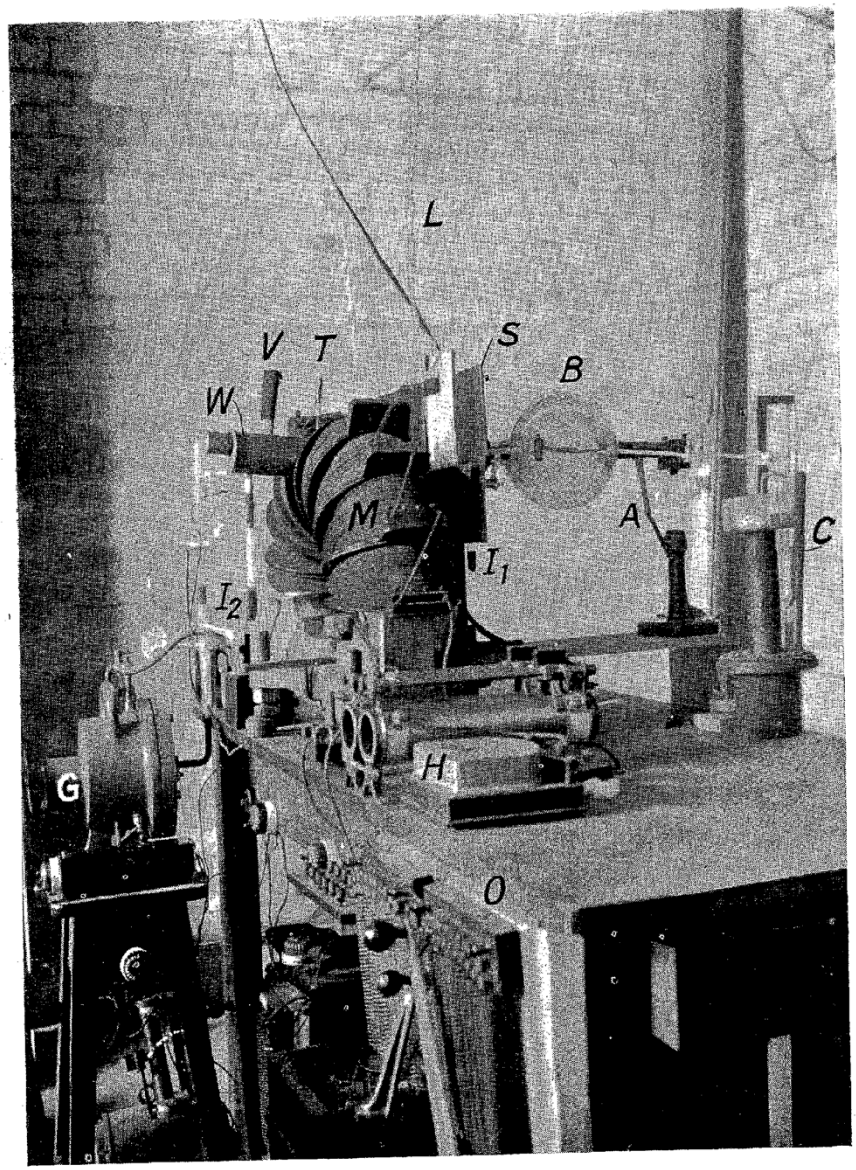
Aston's first "mass spectrograph" from the book (1933):

Mass Spectra and Isotopes

by

FW Aston (Nobel laureate)

Resolution, R=130



THE ORIGINAL MASS SPECTROGRAPH SET UP IN THE CAVENDISH LABORATORY IN 1919; NOW IN THE SCIENCE MUSEUM, SOUTH KENSINGTON.

B, Discharge Tube. *A*, Anode connected to high potential terminal of induction coil below table. *C*, Reservoir containing gas to be analysed. I_1, I_2, Charcoal-liquid air tubes exhausting slit-system and camera. *S*, Soft iron plates to shield discharge from stray magnetic field. *L*, Leads from high tension battery to electric plates. *M*, Du Bois electromagnet. *T*, Pea lamp for photographing fiducial spot. *V*, Vacuum-tight and light-tight control for moving photographic plate. *W*, Camera showing light-tight cap on the left. *H*, Magnet circuit ammeter. *O*, Magnet circuit control resistances. *G*, Gaede rotating mercury pump connected to the camera and the discharge tube by glass tubes and stopcocks.

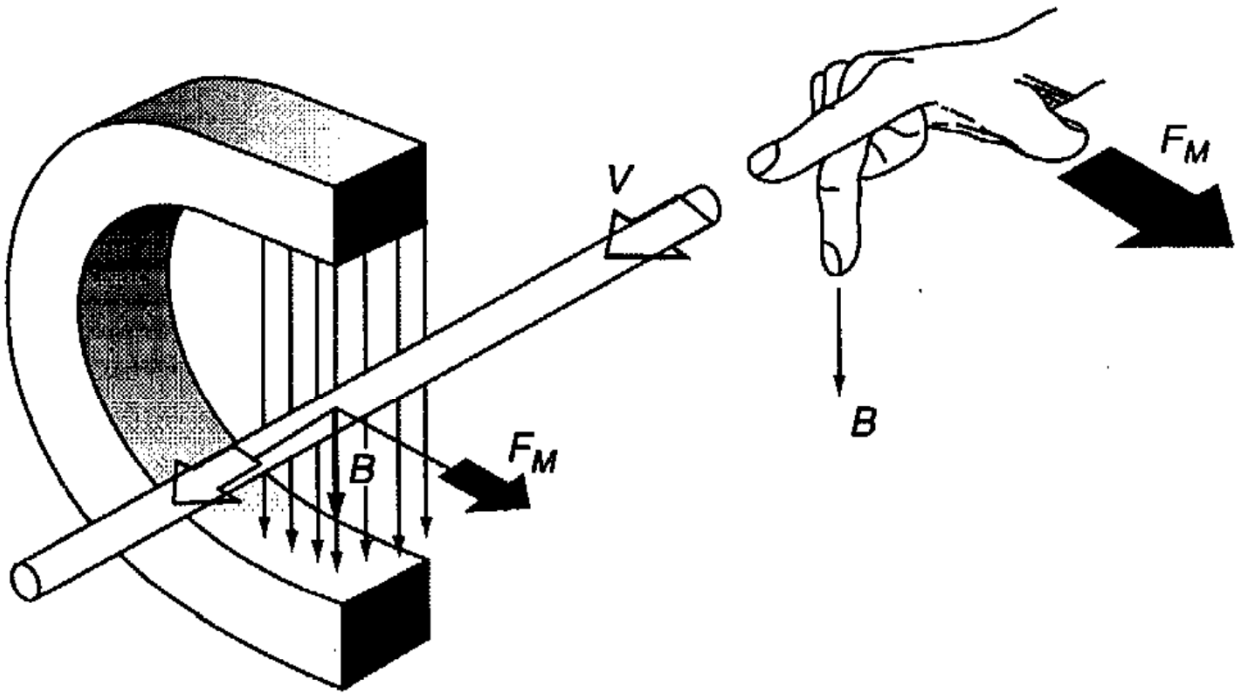


Figure 2.48
Orientation of the magnetic force on a moving ion.

ions at the source outlet leads to

$$mv^2 = 2qV_s$$

Hence

$$\frac{m}{q} = \frac{r^2B^2}{2V_s}$$

Each mass has a different radius. Compare prism and light

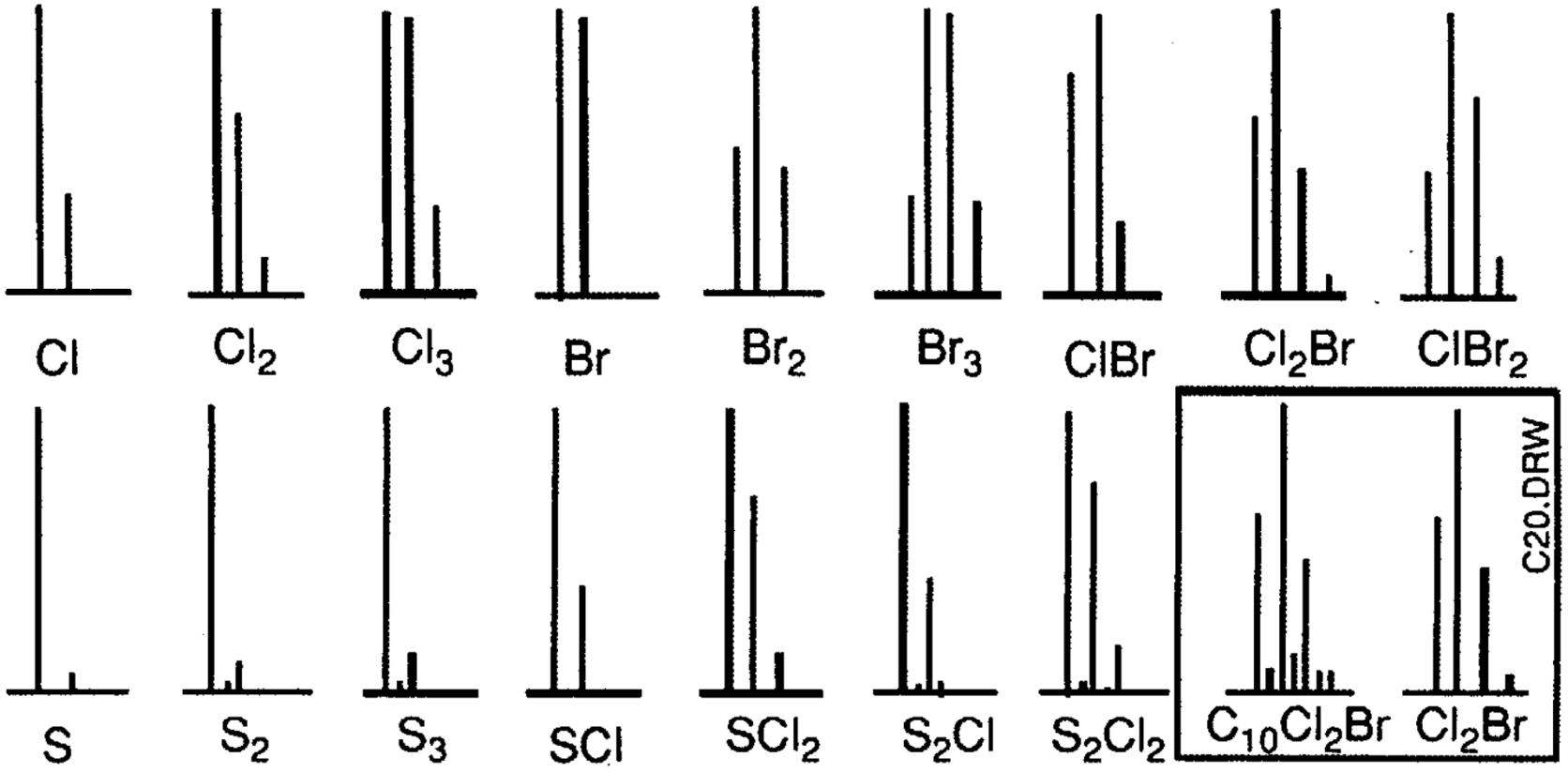


Figure 6.7
Useful isotope combinations in mass spectrometry. Isotopes of other atoms that are possibly associated must always be taken into account, as is shown in the framed section.

Table 6.1 Isotopic abundances.

Isotope	Relative abundance (%)	Mass (u)	Mean atomic mass[a]	
			Calculated	Measured
^{1}H	99.985	1.007 825	1.007 976	1.007 94
^{2}H	0.015	2.014 0		
^{12}C	98.90	12.000 000	12.011 036	12.011 1
^{13}C	1.10	13.003 355		
^{14}N	99.63	14.003 074	14.006 762	14.006 74
^{15}N	0.37	15.000 108		
^{16}O	99.76	15.994 915	15.999 324	15.999 43
^{17}O	0.04	16.999 131		
^{18}O	0.20	17.999 160		
^{19}F	100	18.998 403	18.998 403	18.998 4
^{23}Na	100	22.989 767	22.989 767	22.989 76
^{31}P	100	30.973 762	30.973 762	30.973 76
^{32}S	95.02	31.972 070	32.064 385	32.066 6
^{33}S	0.75	32.971 456		
^{34}S	4.21	33.967 866		
^{36}S	0.02	35.967 080		
^{35}Cl	75.77	34.968 852	35.452 737	35.452 79
^{37}Cl	24.23	36.965 903		
^{39}K	93.2581	38.963 707	39.098 299	39.098 31
^{40}K	0.0117	39.963 999		
^{41}K	6.7302	40.961 825		
^{79}Br	50.69	78.918 336	79.903 526	79.904 1
^{81}Br	49.31	80.916 289		

[a] Mean value for the natural mixture of isotopes.

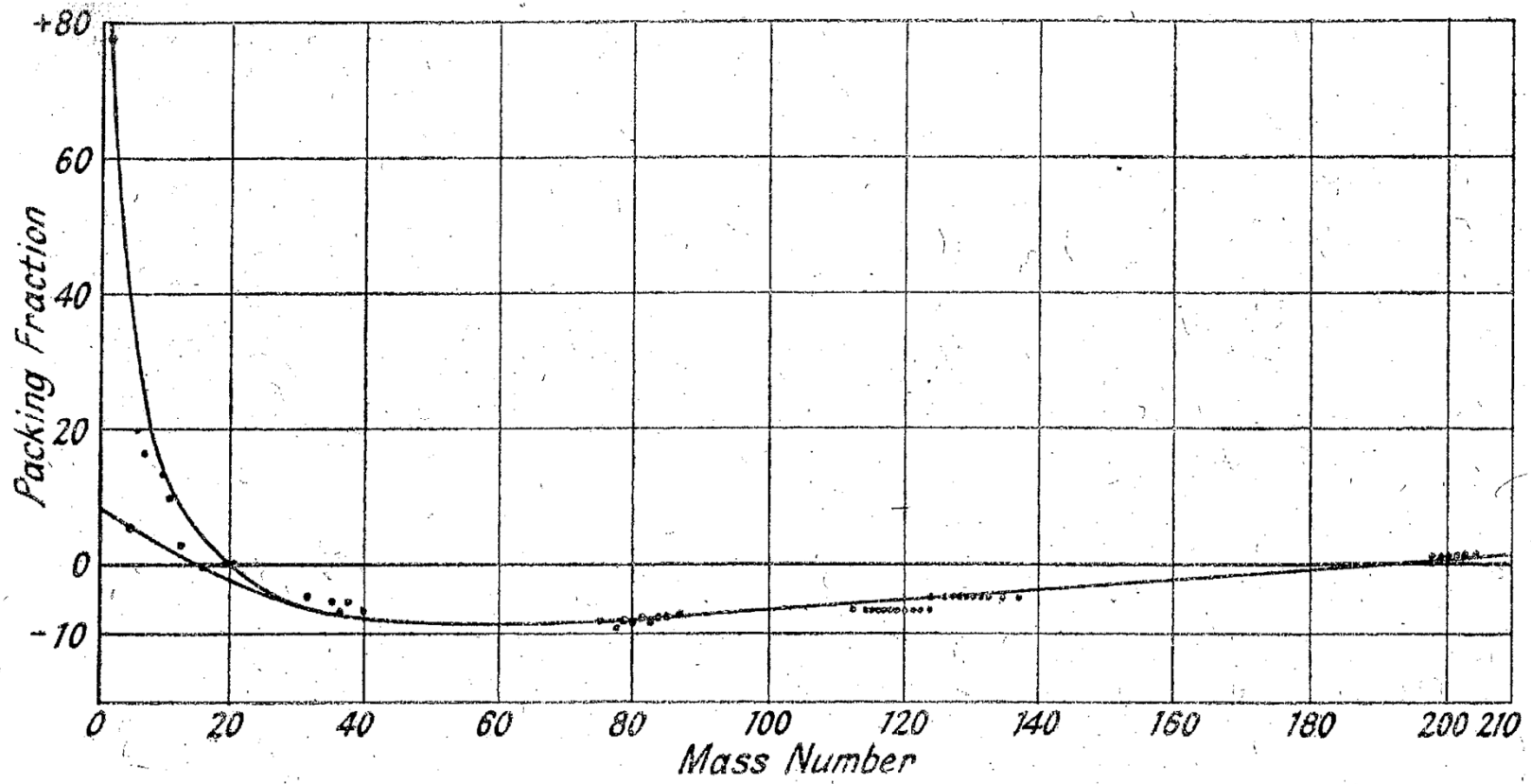
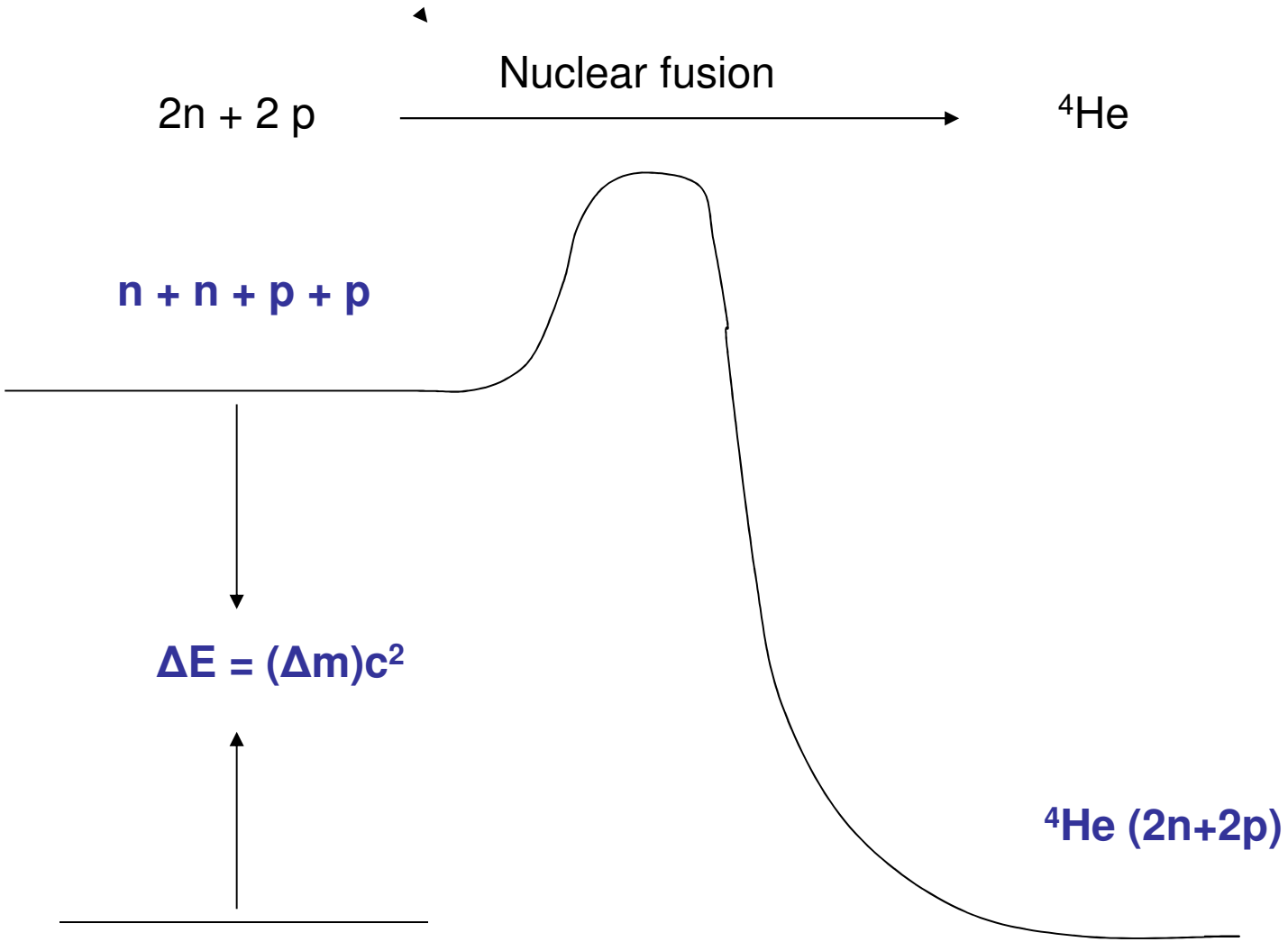


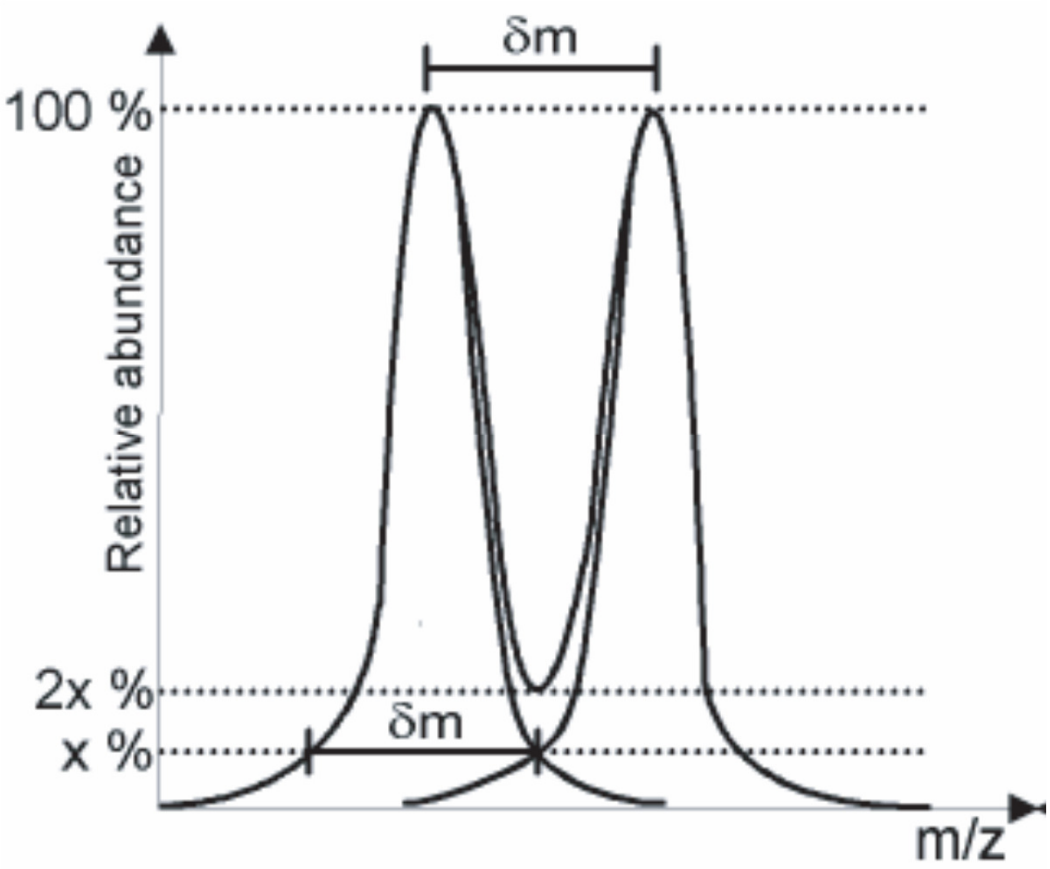
FIG. 20.—Aston's Original Packing Fraction Curve (1927).

From the book (1933): Mass Spectra and Isotopes
by
FW Aston (Nobel laureate)

Origin of mass defect in mass spectrometry – nuclear binding

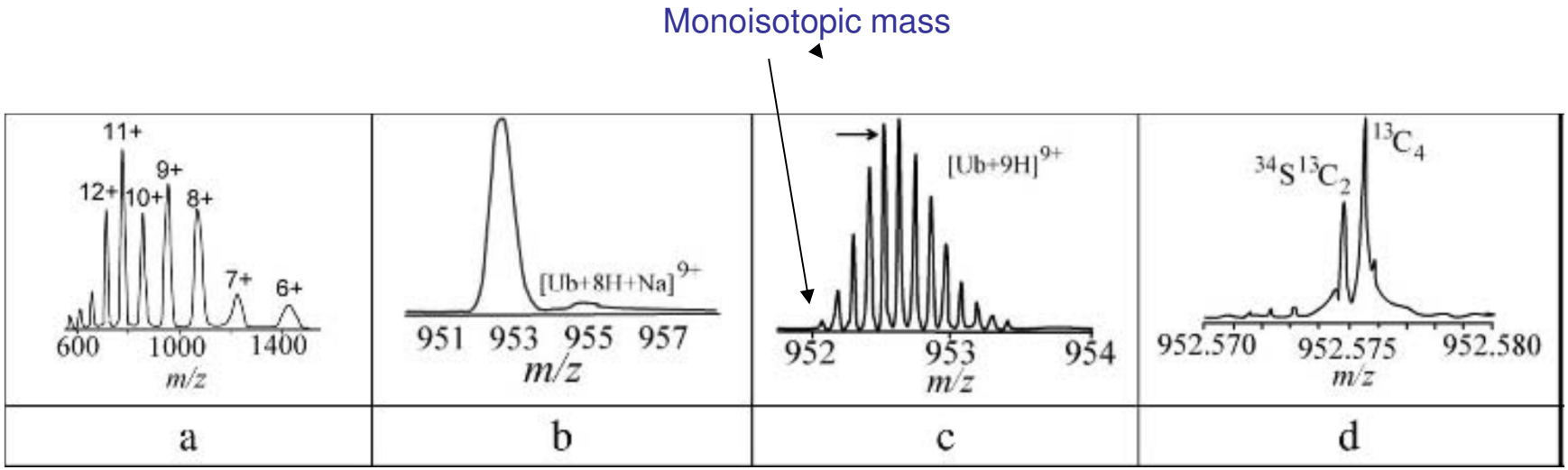


RESOLVING POWER: $R = m/\delta m$ (20% valley) if our criterion is say 20% valley between peaks before we term peaks resolved. (The RESOLUTION in this case is δm)



$R = m/\delta m$ with δm measured from two peaks resolved at say 20% valley or from the width of one peak at 10% peak height.

An illustration of the information attainable with increasing resolving power R: R(a) > 100; R(b) > 1000; R(c) > 10,000 and R(d) > 100,000



Increasing the resolving power for the detection of peaks from ubiquitin (C378H630N105O118S).Redrawn from data in Marshall A.G., Hendrickson C.L. and Shi S.D.H., Anal. Chem., 74, 253A–259A, 2002.
The resolving power shown in d is around 500,000

Increase in MS resolution over a century

Year	R=m/Δm	Authors
• 1913	13	Thomson
• 1918	100	Dempster
• 1919	130	Aston
• 1937	2000	Aston
• 1998	8 000 000	Marshall & co

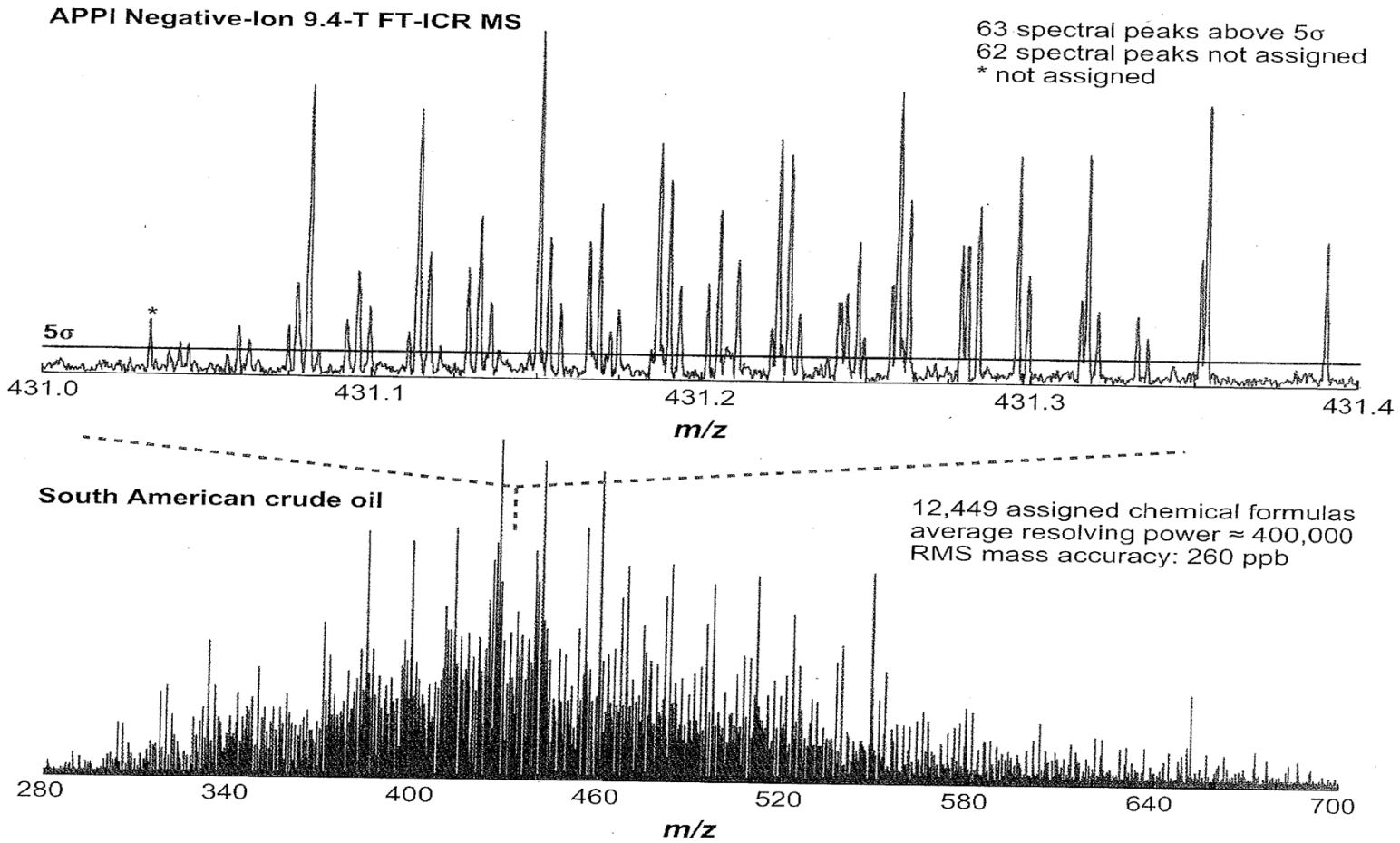


Figure 7

Atmospheric pressure photoionization negative ion 9.4-T Fourier transform–ion cyclotron resonance (FT-ICR) mass spectrum of a South American crude oil, showing the largest total number (and largest number spanning one Dalton) of assigned elemental compositions published to date. Figure adapted with permission from Reference 73.

Alan Marshall

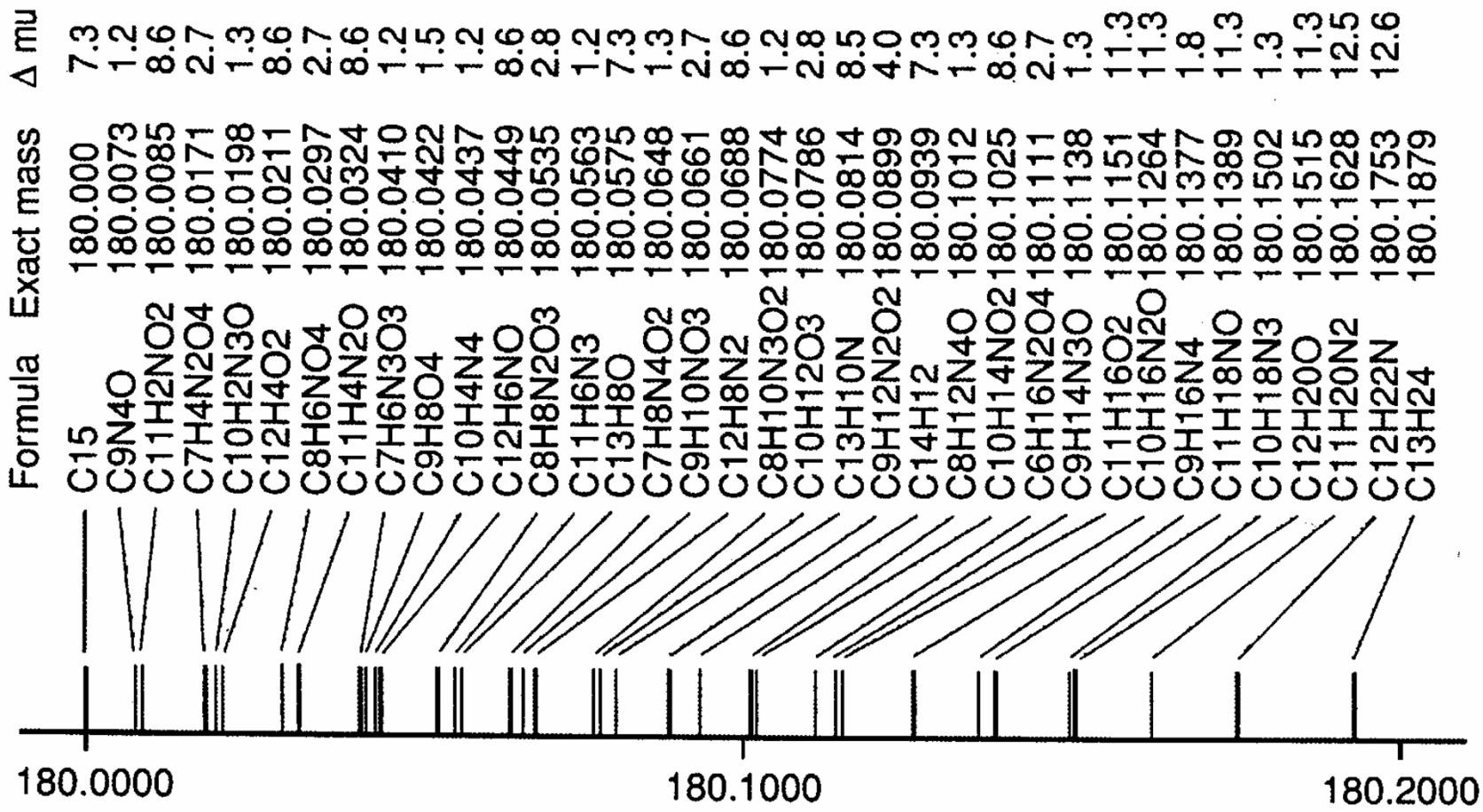
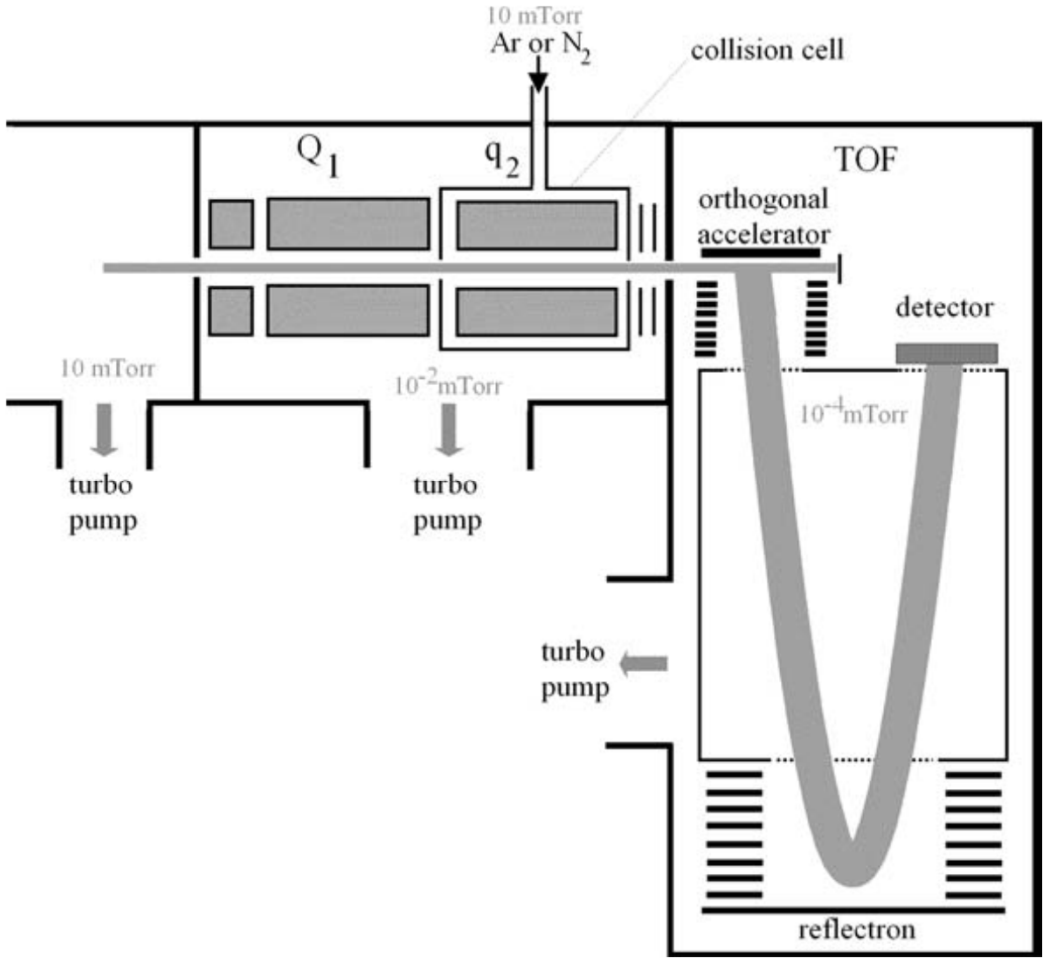
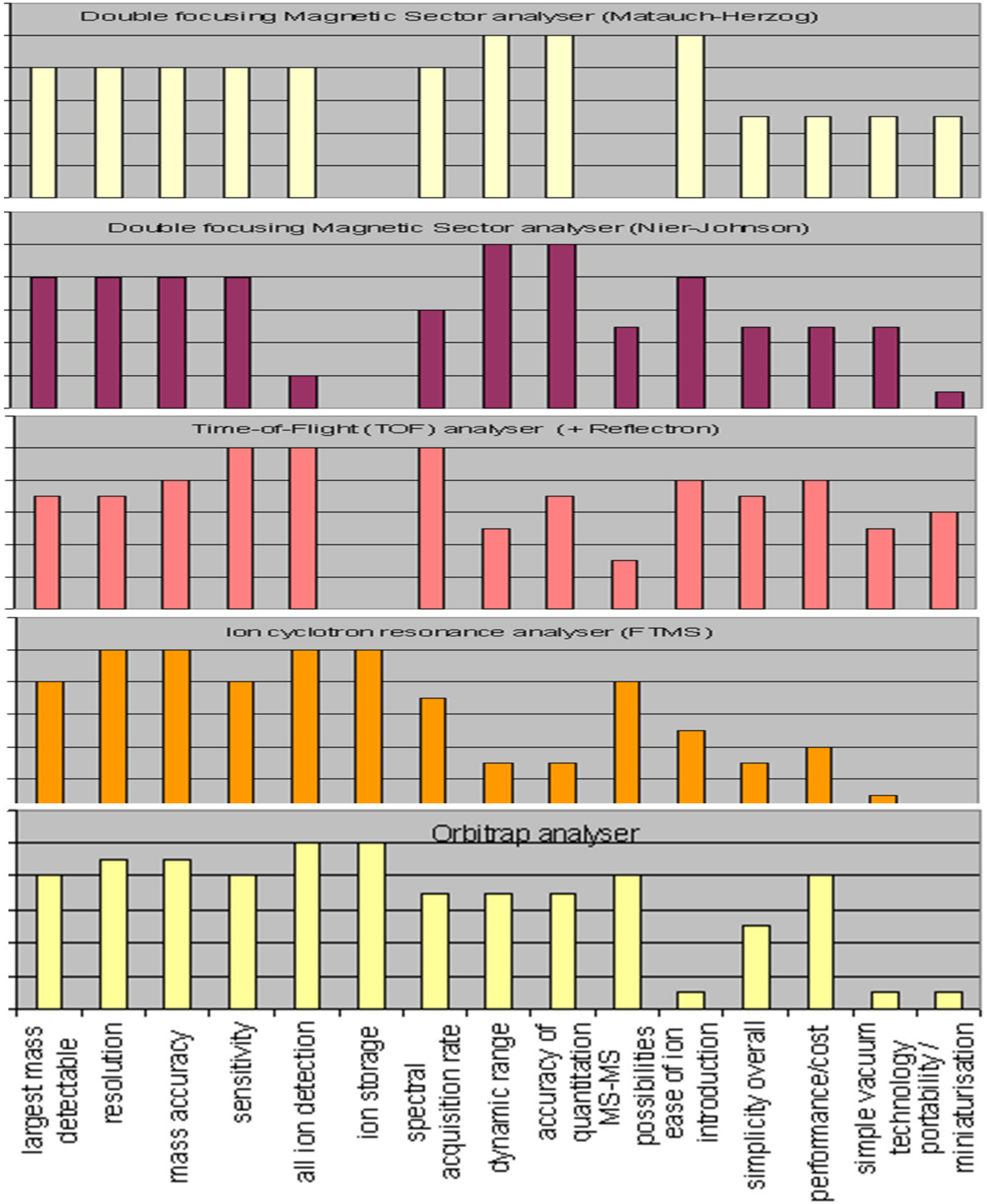


Figure 6.3
Exact masses and corresponding formulae for various possible ions of *m/z* 180 containing only carbon, hydrogen, nitrogen and oxygen atoms in limited number (C_{6-15}, H_{0-24}, N_{0-4} and O_{0-4}).

Mass Spectrometry 3rd ed, De Hoffman

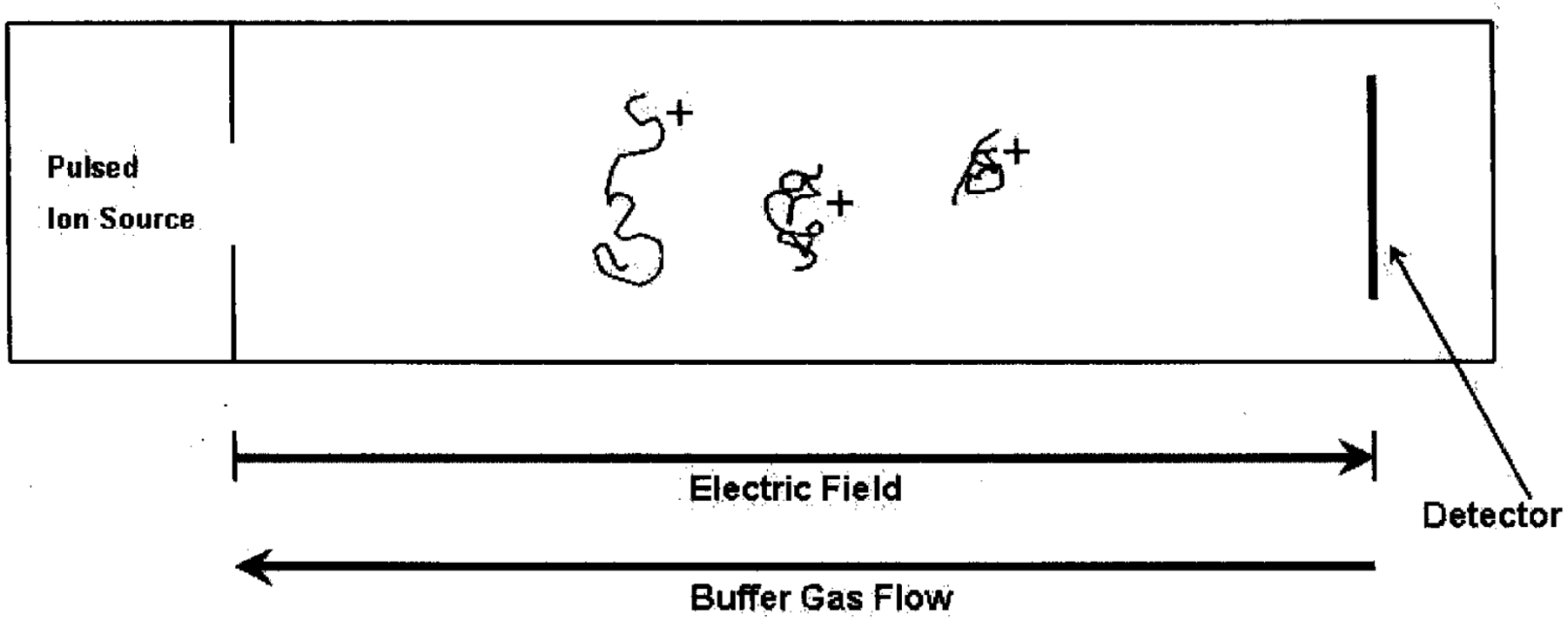
MS-MS via Q-TOF analysers




Double focusing Magnetic Sector analyser (Matauch-Herzog)
Double focusing Magnetic Sector analyser (Nier-Johnson)
Time-of-Flight (TOF) analyser (+ Reflectron)
Ion cyclotron resonance analyser (FTMS)
Orbitrap analyser
largest mass detectable
resolution
mass accuracy
sensitivity
all ion detection
ion storage
spectral acquisition rate
dynamic range
accuracy of quantitation
MS-MS possibilities
ease of ion introduction
simplicity overall
performance/cost
simple vacuum technology
portability/ miniaturisation

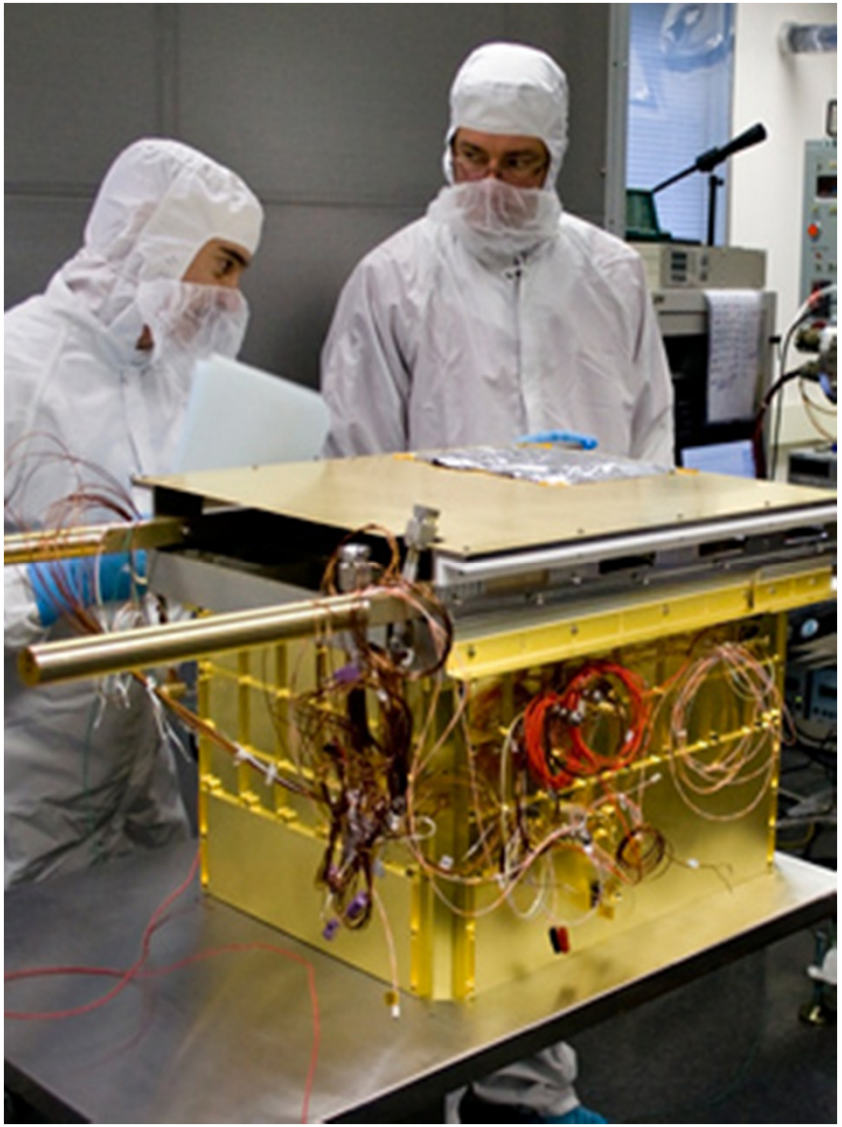
High definition MS ?

Ion mobility in the millisecond time domain

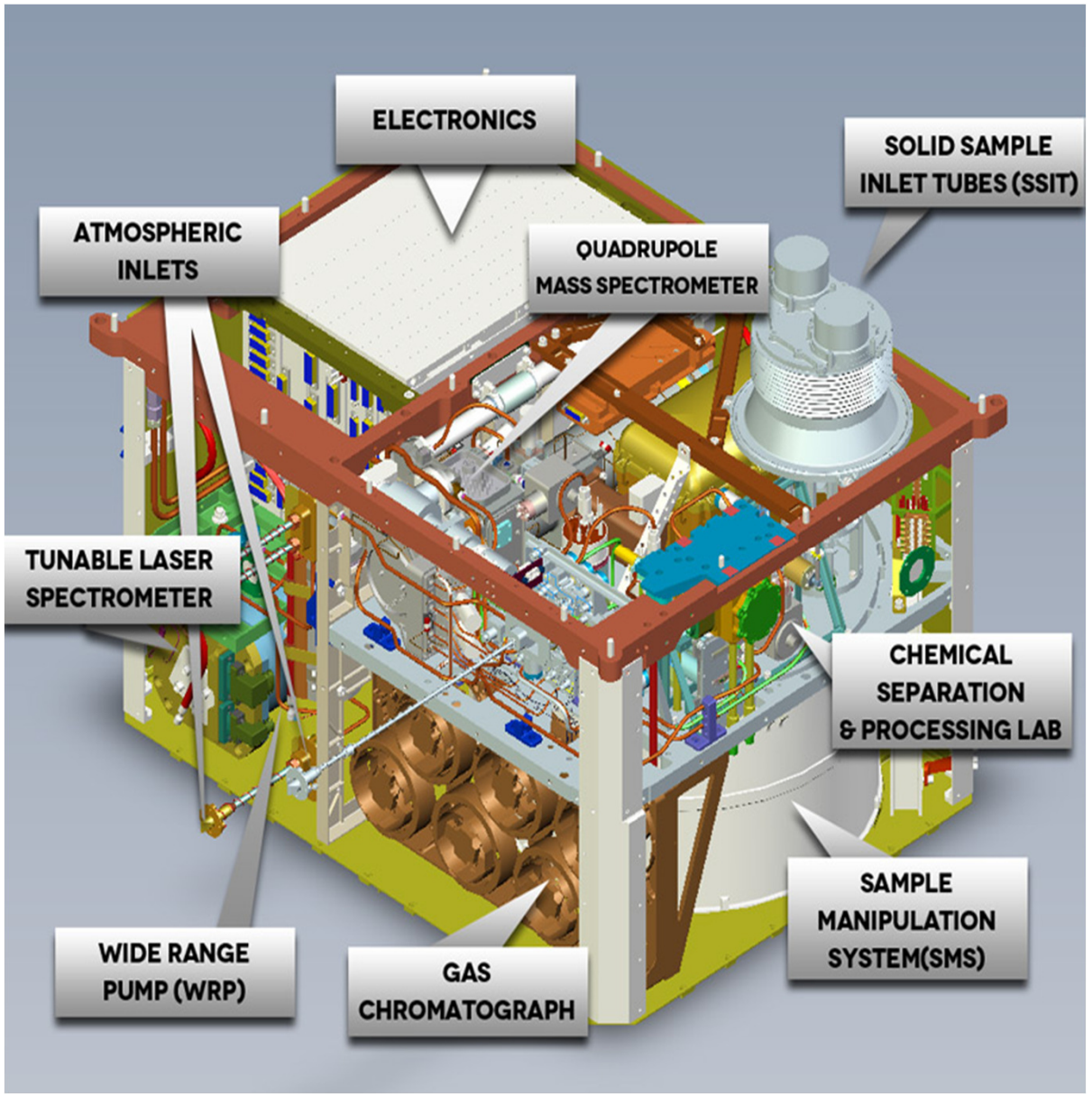


NASA’s Sample Analysis at Mars (SAM) for Curiosity Mars rover

SAM is a suite of three instruments totaling 40 kg, located in the Curiosity rover's interior: a 6-column Gas Chromatograph (GC), a Quadrupole Mass Spectrometer (QMS), and a Tunable Laser Spectrometer (TLS). These instruments are coupled through solid and gas processing systems to provide complementary information on the same samples. Each sample may be analyzed by one, two, or all three of the SAM instruments.



The search for organic molecules is particularly important in the search for life on Mars because life as we know it cannot exist without them (though they can exist without life). SAM will be able to detect lower concentrations of a wider variety of organic molecules than any other instrument yet sent to Mars.



Structure of lecture

- Introduction
- Historical perspective
- Personal research experience, with emphasis on recent years
- Vision for the Department

Phases in my career

- Interest in the fundamentals
- Need to feel useful
- A growing feeling of responsibility

Organic analysis of complex mixtures are a challenge

Literally hundreds and thousands of compounds are present in:

- Natural products
- Petrochemicals
- Aroma of food and beverages
- All trace analysis

These analyses all require combined chromatography – mass spectrometry instrumentation

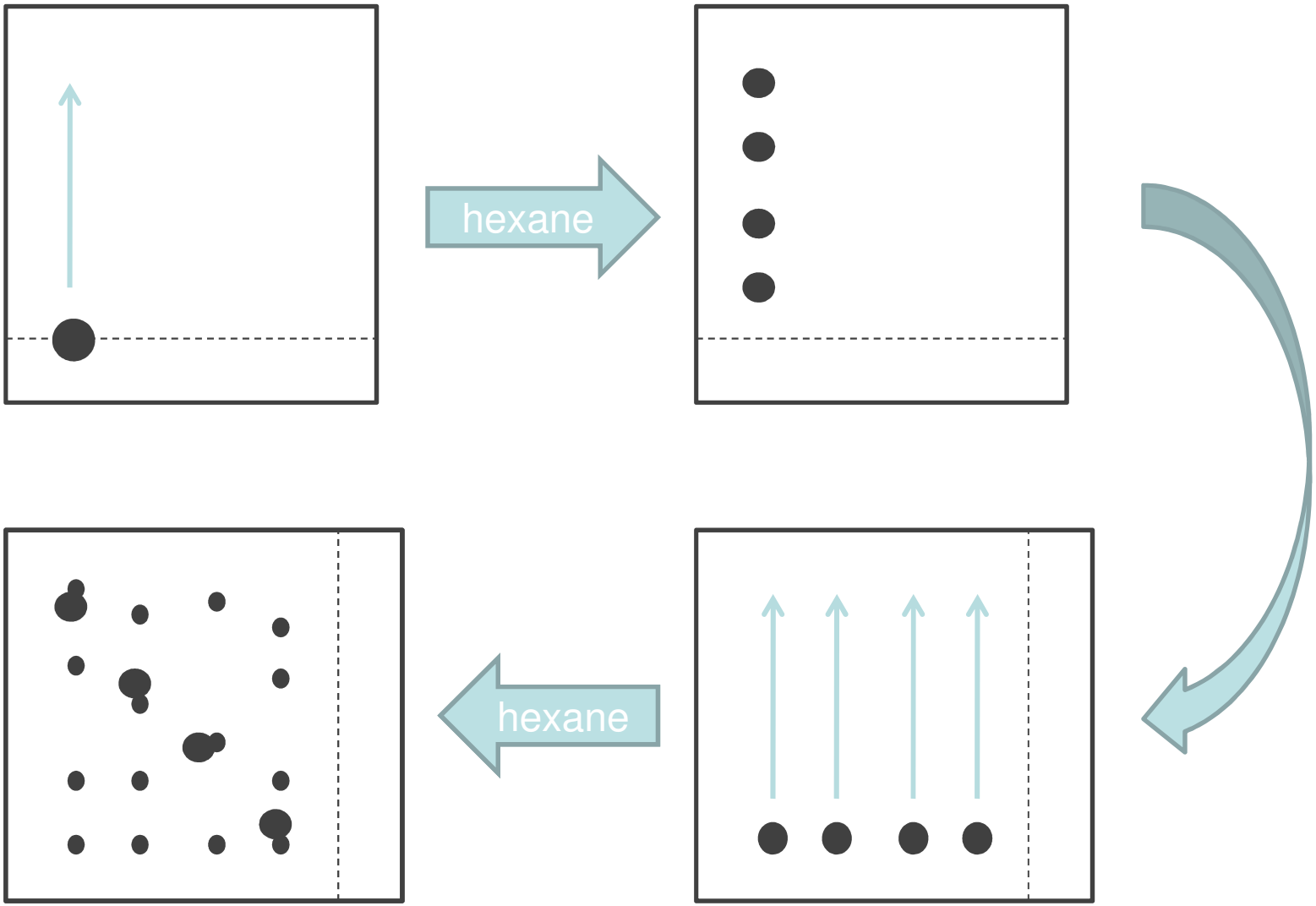
Typical trace analysis consists of:

Concentration **Separation** **Selective detection**

Our research programme addresses all three aspects, trying to improve the sensitivity, selectivity, time and costs.

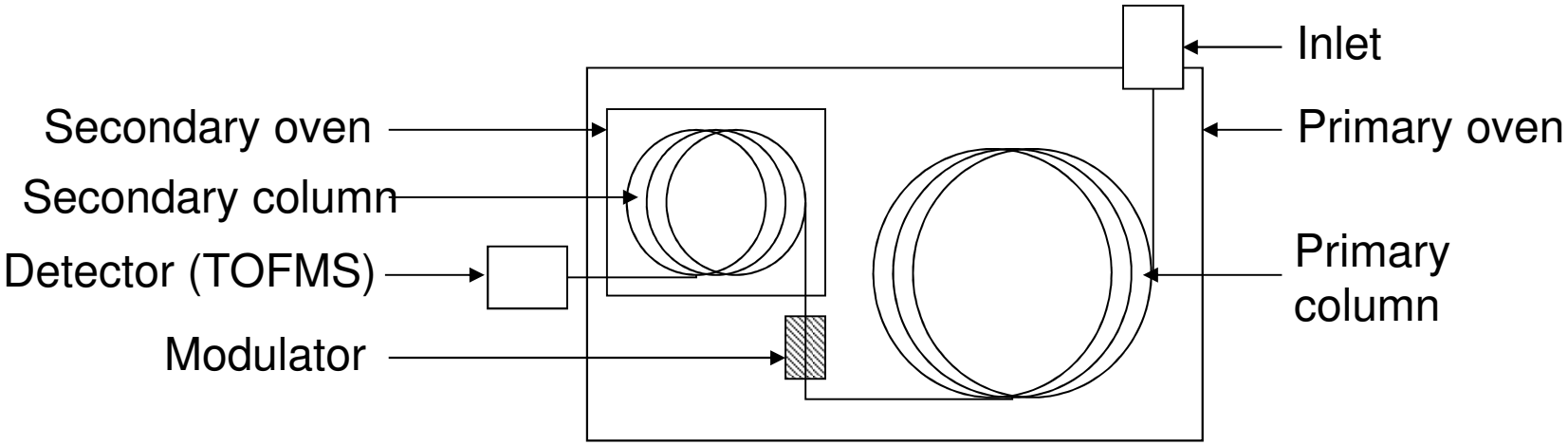
Concentration	**Multichannel silicone rubber traps**
Separation	**Multidimensional chromatography**
Selective detection	**High resolution MS** **Special ionization techniques MS** **Human nose** **Insect antennae**

Two-dimensional separation

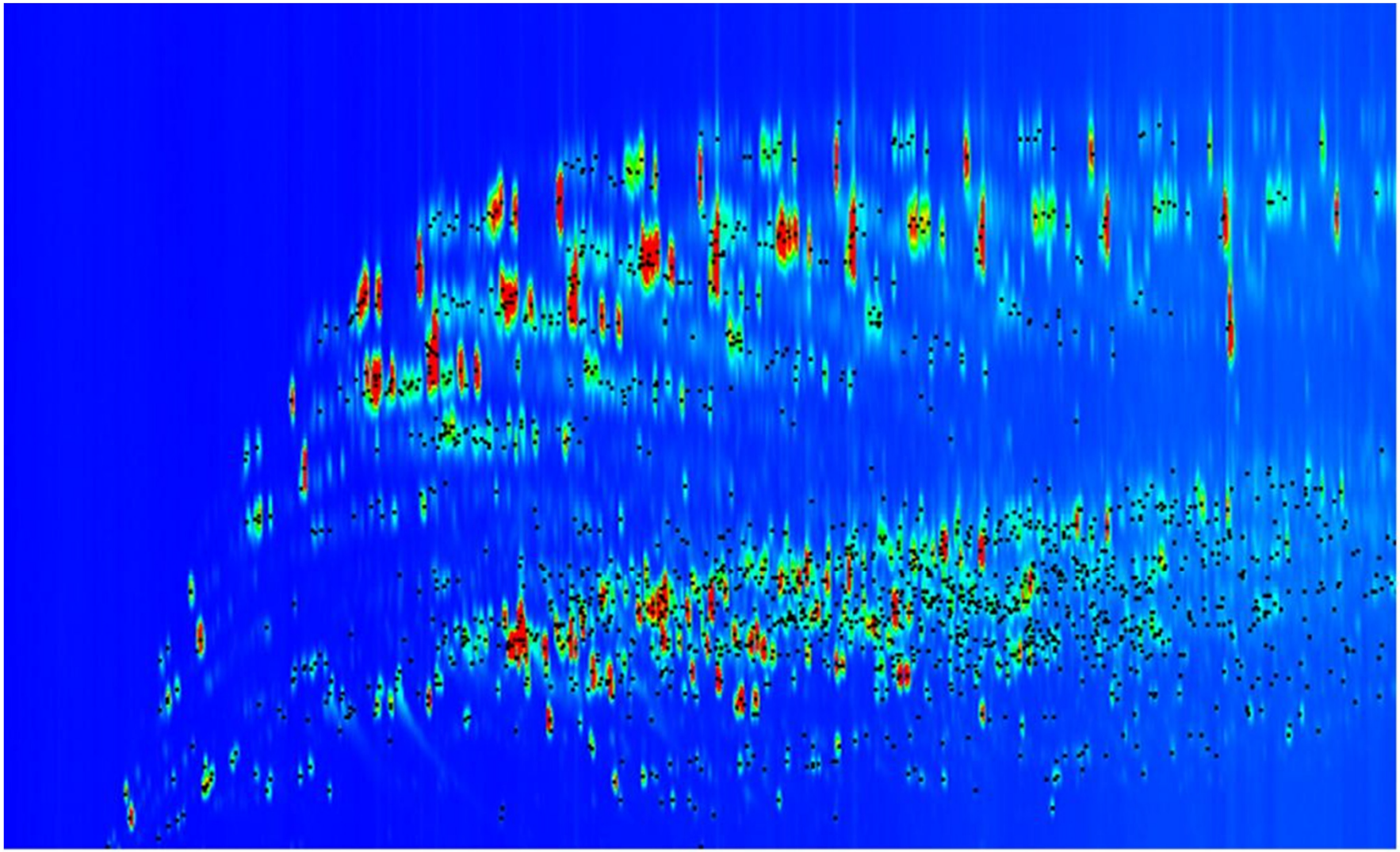


GCXGC/TOFMS

Comprehensive two-dimensional gas chromatography Time-of-flight mass spectrometry

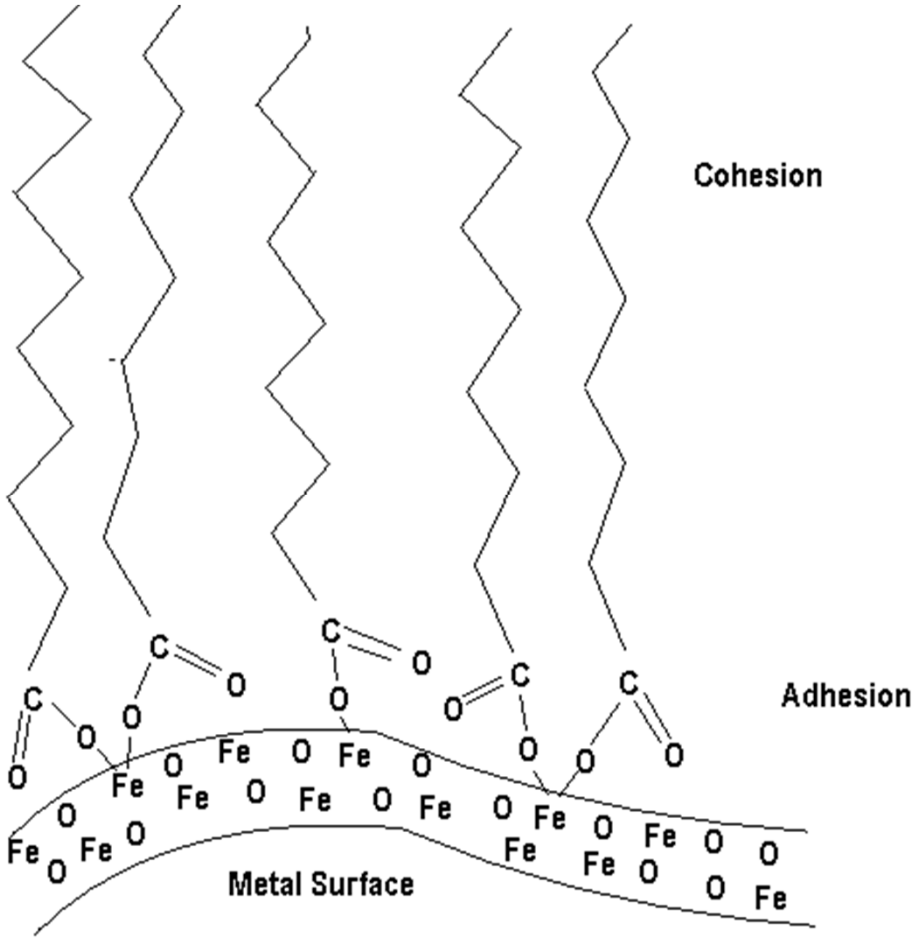


Results: Two-dimensional Chromatogram



Chemisorption

A chemical understanding of Lubricity



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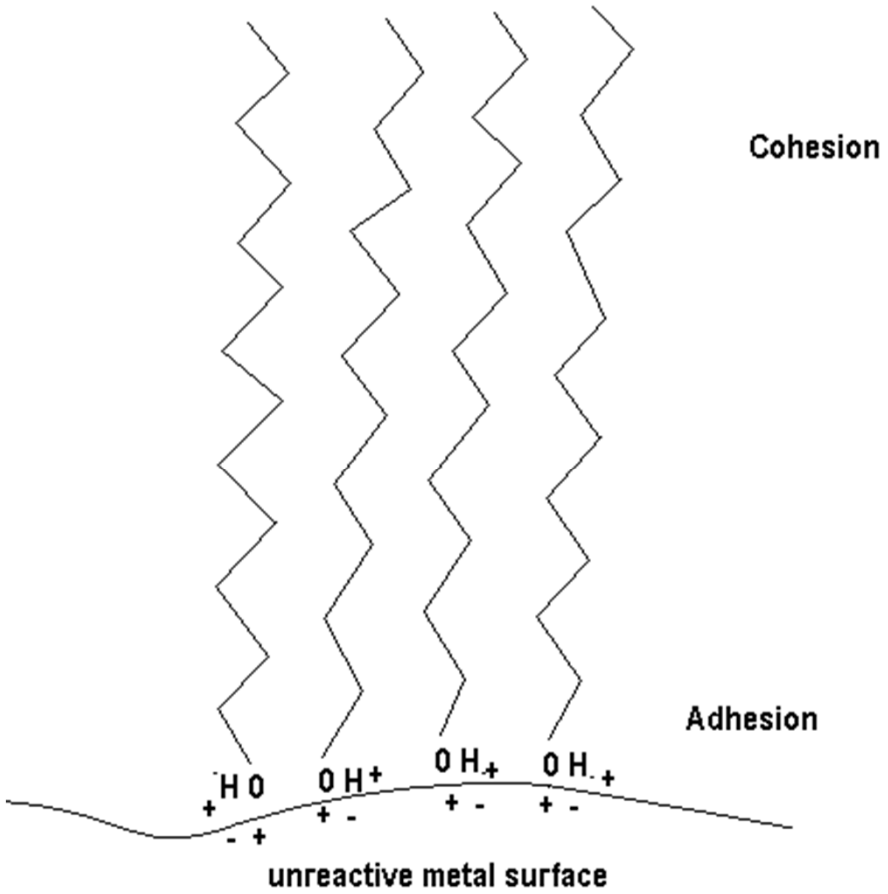

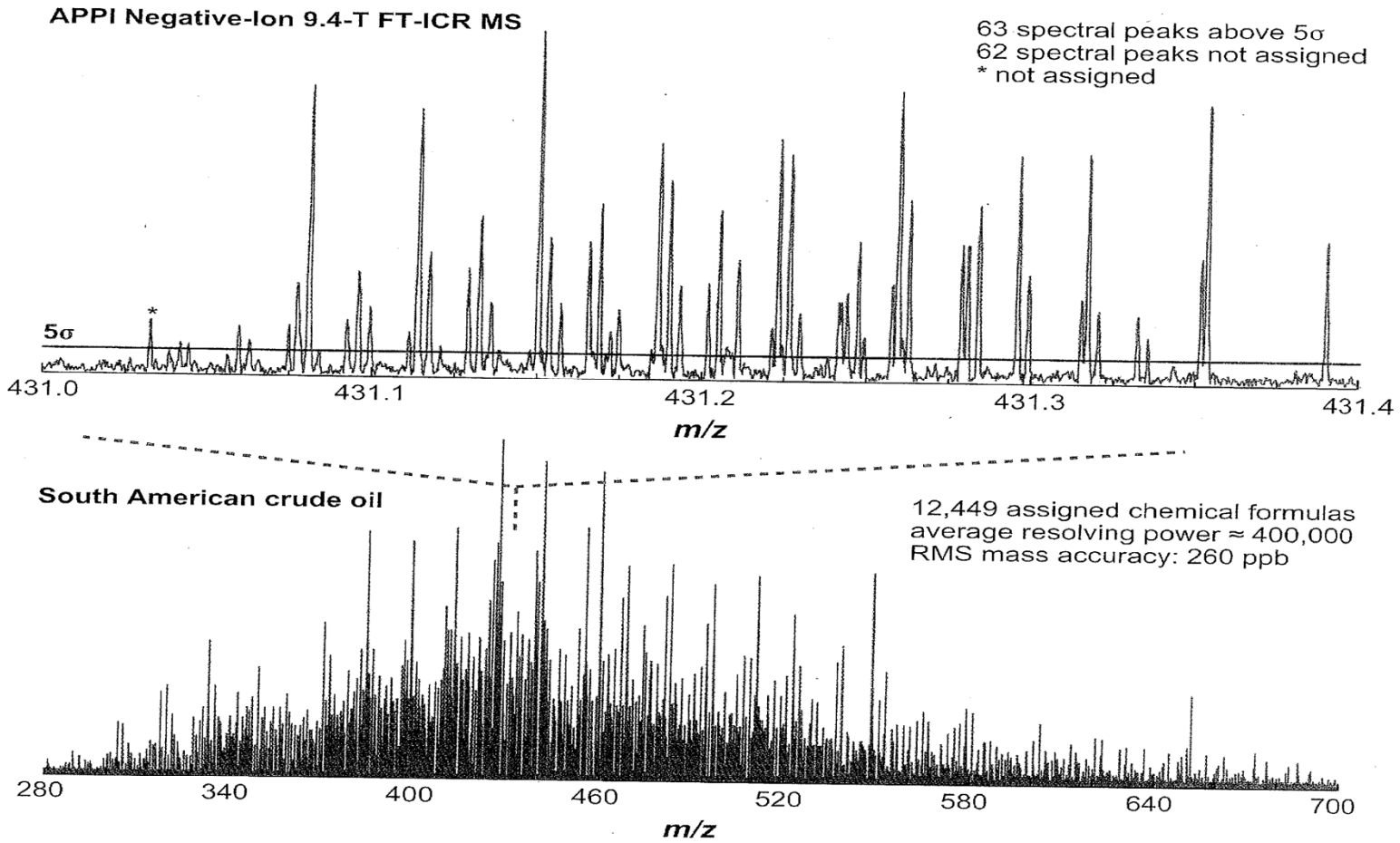

Figure 7

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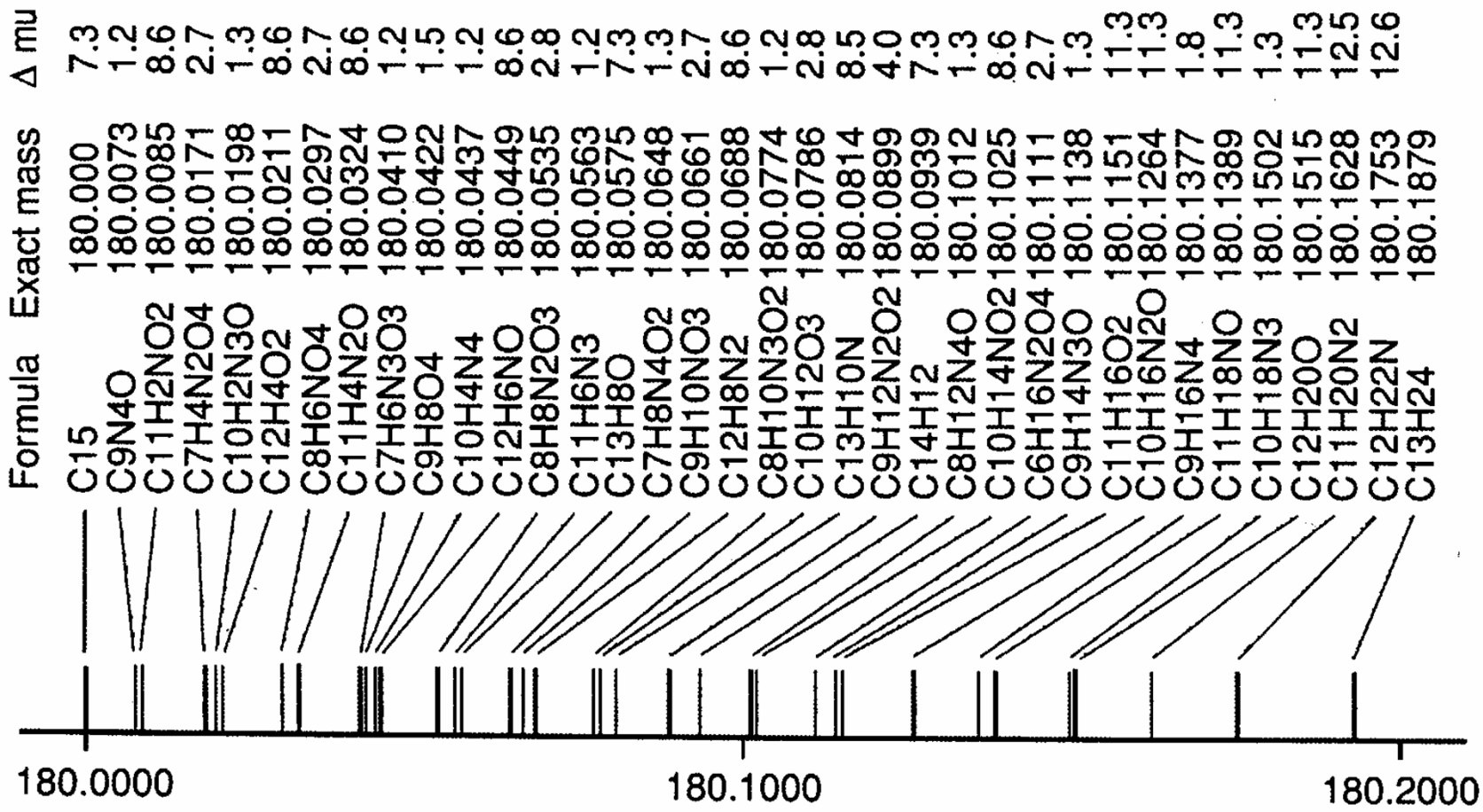

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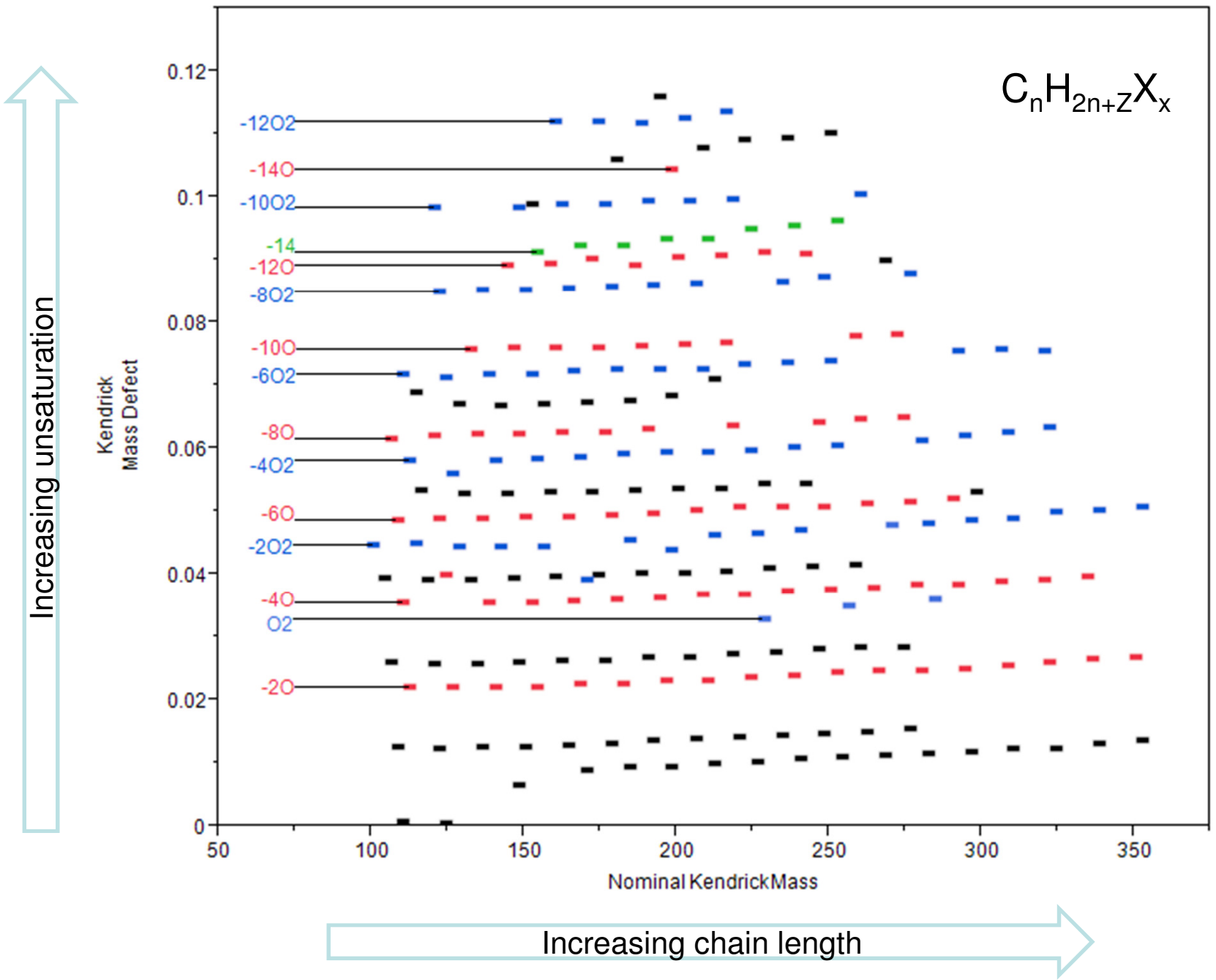
Mass Spectrometry 3rd ed, De Hoffman


$C_nH_{2n+Z}X_x$
Increasing unsaturation
Kendrick Mass Defect
0.12
0.1
0.08
0.06
0.04
0.02
0
-12O2
-14O
-10O2
-14
-12O
-8O2
-10O
-6O2
-8O
-4O2
-6O
-2O2
-4O
O2
-2O
50
100
150
200
250
300
350
Nominal Kendrick Mass
Increasing chain length

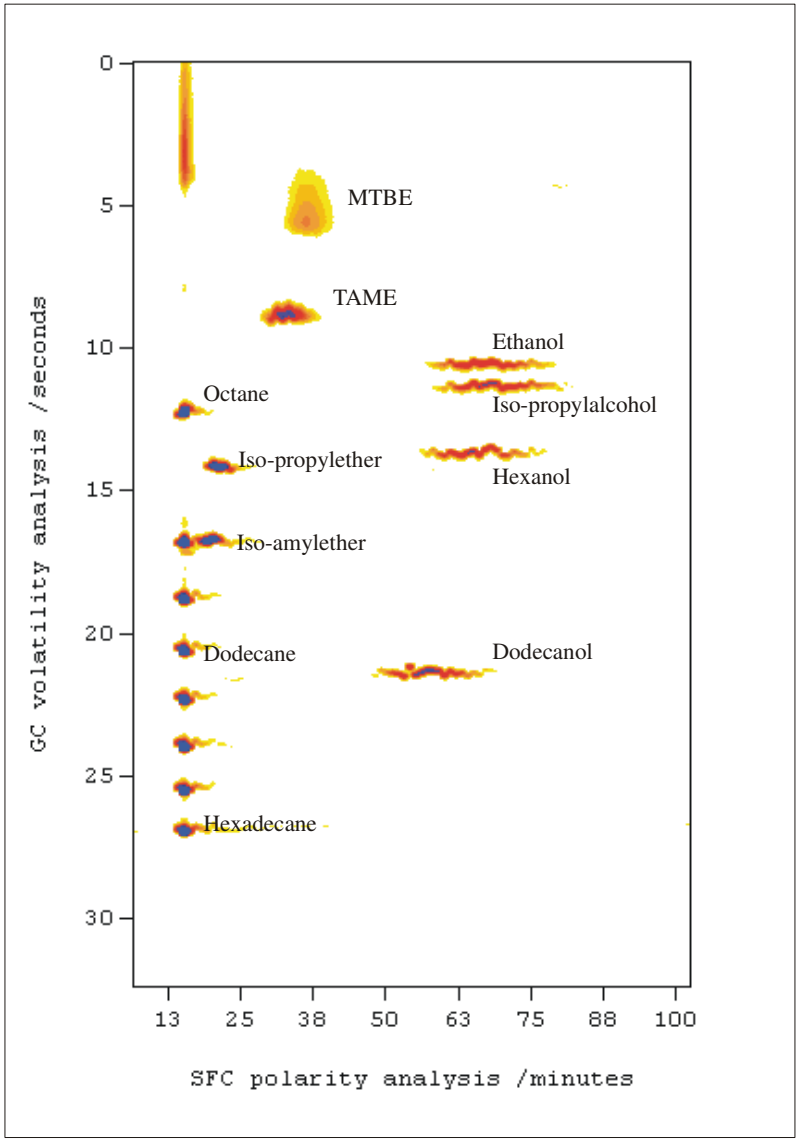


Figure 4: SFCxGC analysis of an petrochemical standard containing alkanes, ethers and alcohols. CO_2 at a pressure of 150 atm and a temperature of 28°C was used as mobile phase in the SFC analysis. The flow through the PLOT column was collected for intervals of 5 seconds. The GC was repeatedly temperature programmed from -50 to 250°C at 450 °C/min while hydrogen was supplied as carrier gas to obtain a linear flow rate of 1m/sec.

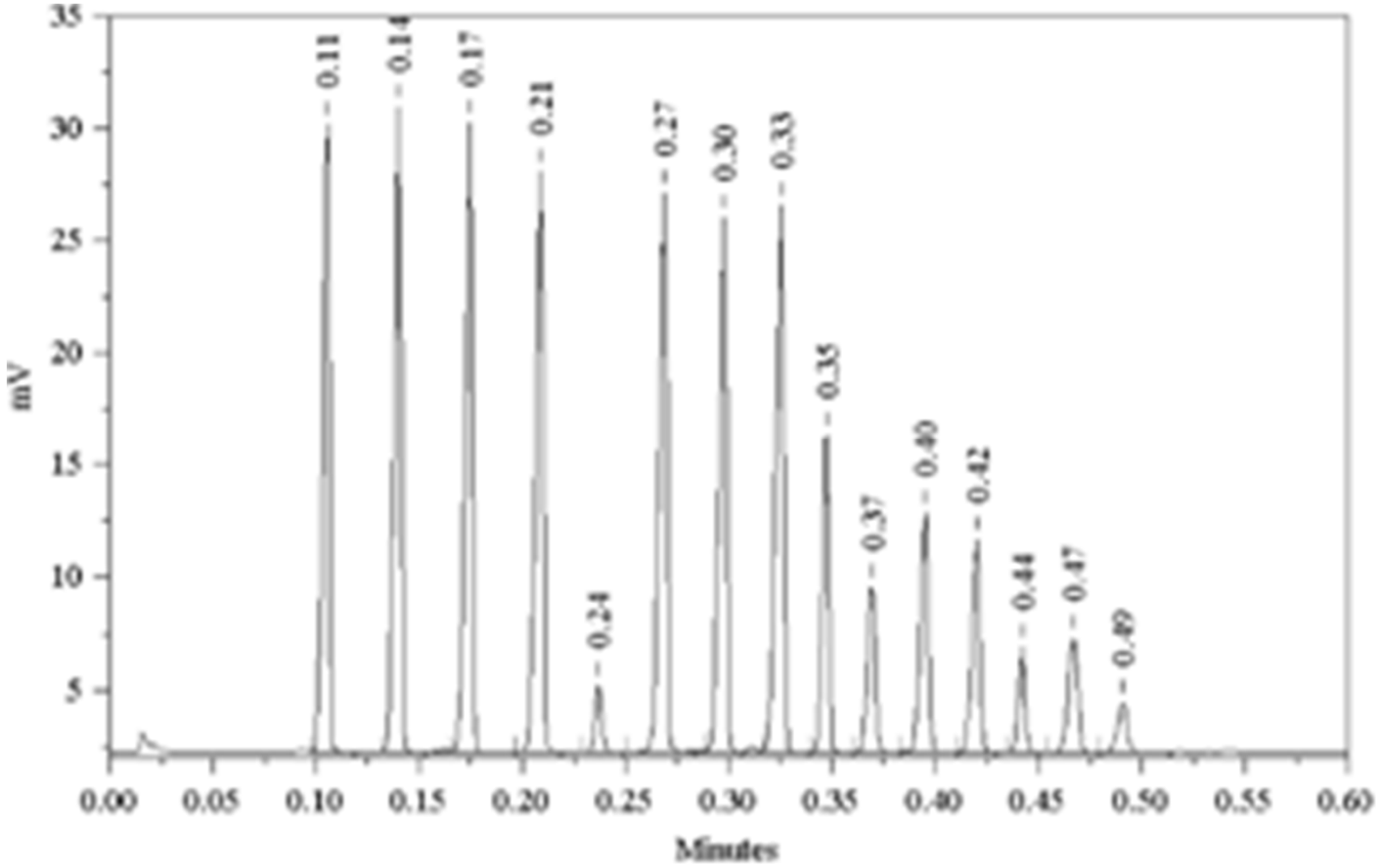
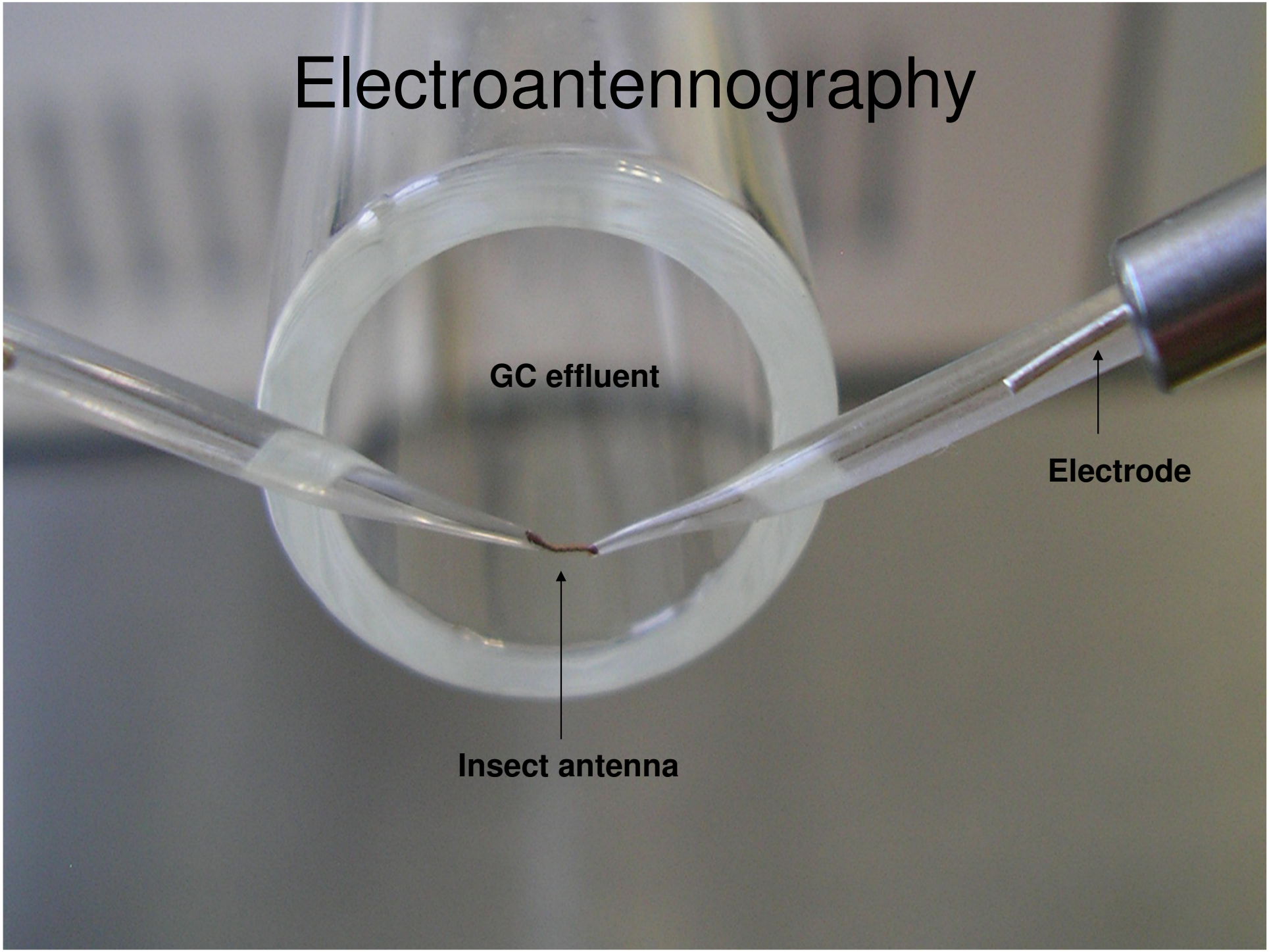


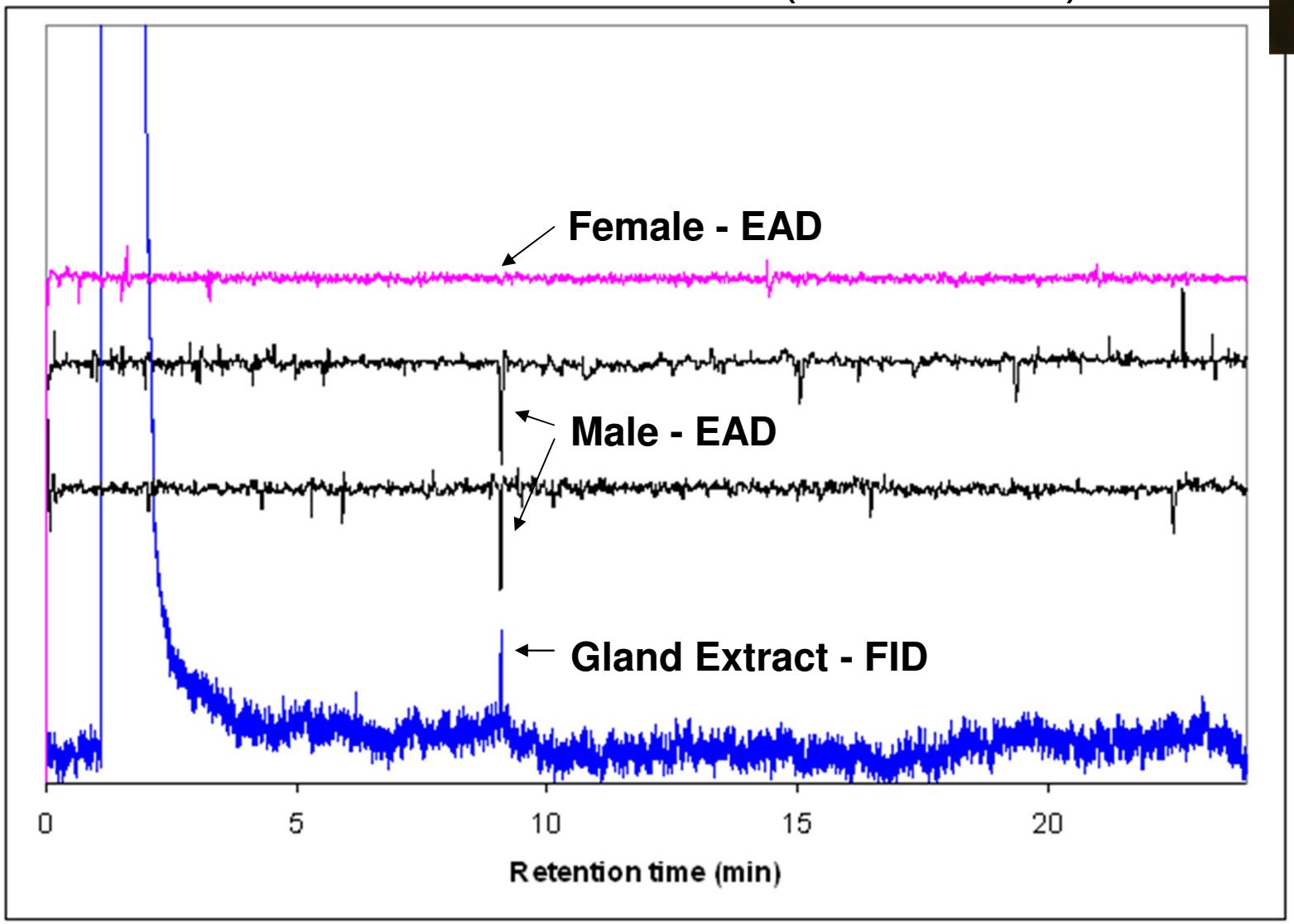
Figure 3. Gas chromatogram obtained at the optimum ramp rate where the maximum attainable separation of the analytes was attained in the shortest time. The sample contained n-alkanes from decane to tetracosane. The temperature was ramped from 50 to 300 ℃. A ramp rate of 450 ℃/min at a flow rate of 100 cm/s was used. Peak capacity of 60 peaks in 30 seconds

Electroantennography



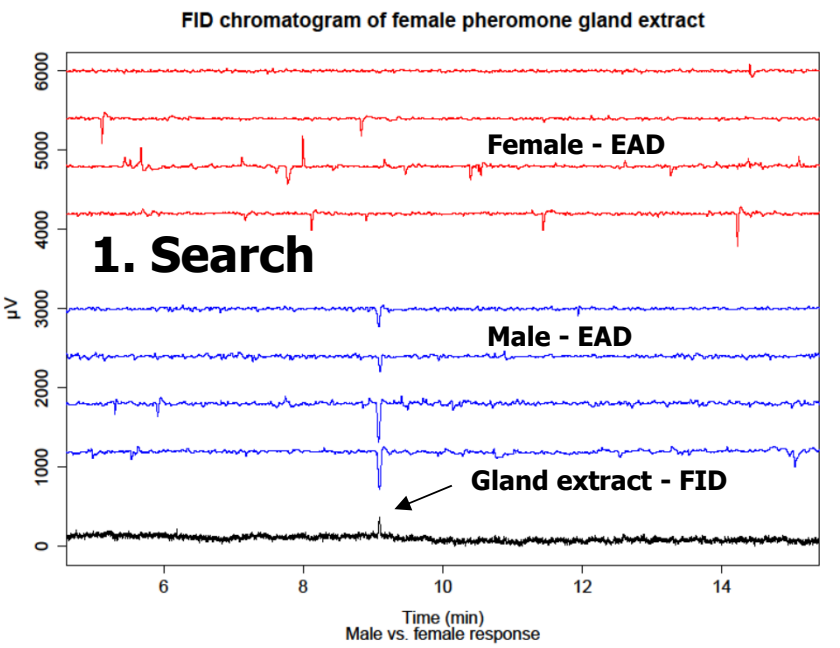
Electroantennography

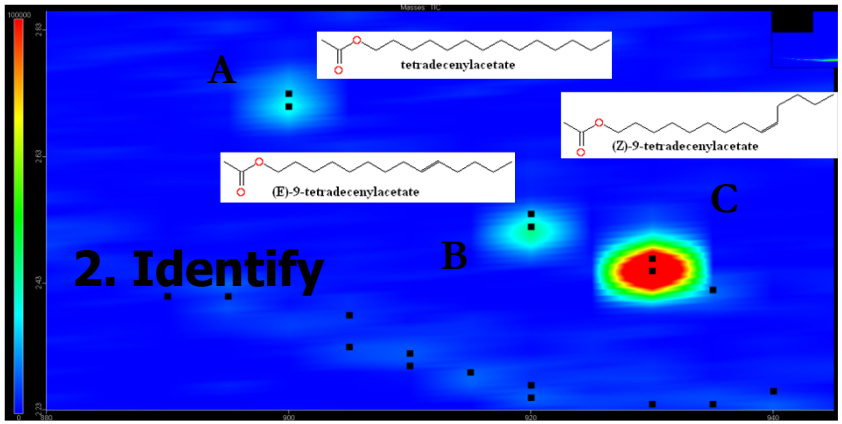
Male vs. Female (40-300°C)



Cossid moth

Pheromones


FID chromatogram of female pheromone gland extract
Female - EAD
1. Search
Male - EAD
Gland extract - FID
µV
0
1000
2000
3000
4000
5000
6000
6
8
10
12
14
Time (min)
Male vs. female response


A
tetradecenylacetate
(Z)-9-tetradecenylacetate
(E)-9-tetradecenylacetate
C
B
2. Identify


3. Behaviour


4. Field trial
-female control

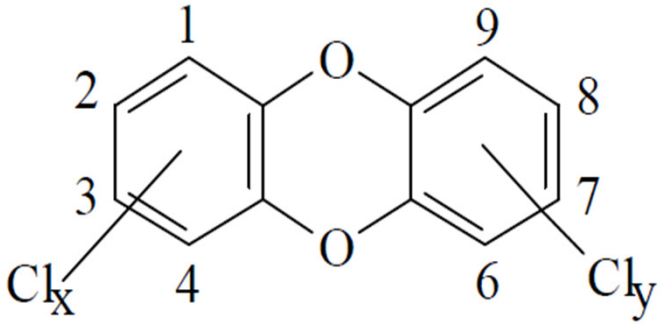
What are Persistent organic pollutants (POPs)?

- POPs are chemical substances that persist in the environment, bio-accumulate through the food web, and pose a risk of causing adverse effects to human health and the environment at locations near and far from their source
- They are typically characterized as having low water solubility and high fat solubility, they are prone to long range transport and most of them are anthropogenic in origin

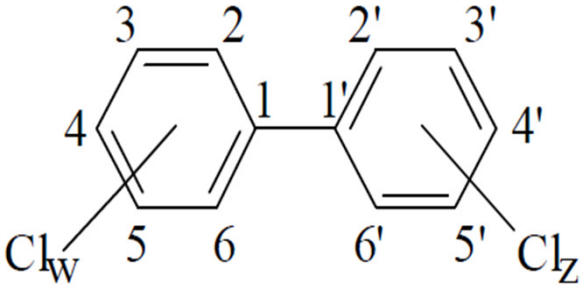
The POP group includes, amongst others, twelve substances ('the dirty dozen"):

- aldrin, chlordane, 2,2-bis(4-chlorophenyl)-1,1,1-trichloroethane (DDT), dieldrin, endrin, heptachlor, hexachloro benzene (HCB), mirex and toxaphene;
- Three are *industrial substances* - polychlorinated biphenyls (PCBs), polychlorinated dibenzo-*p*-dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs)

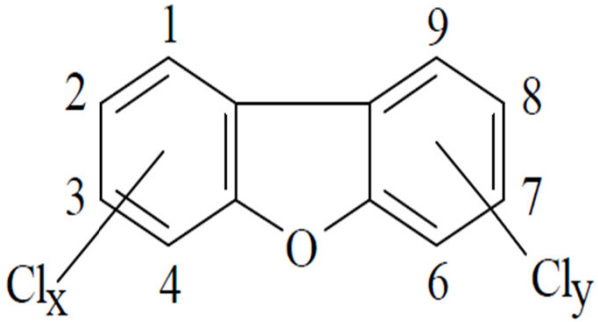
“Dioxin”
PCDDs

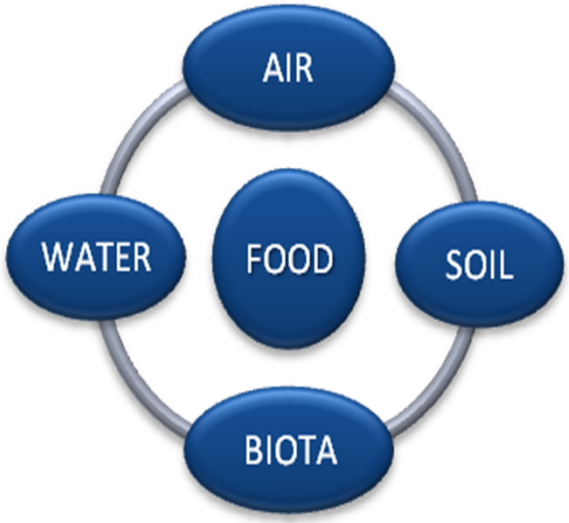


PCBs



“Furan”
PCDFs





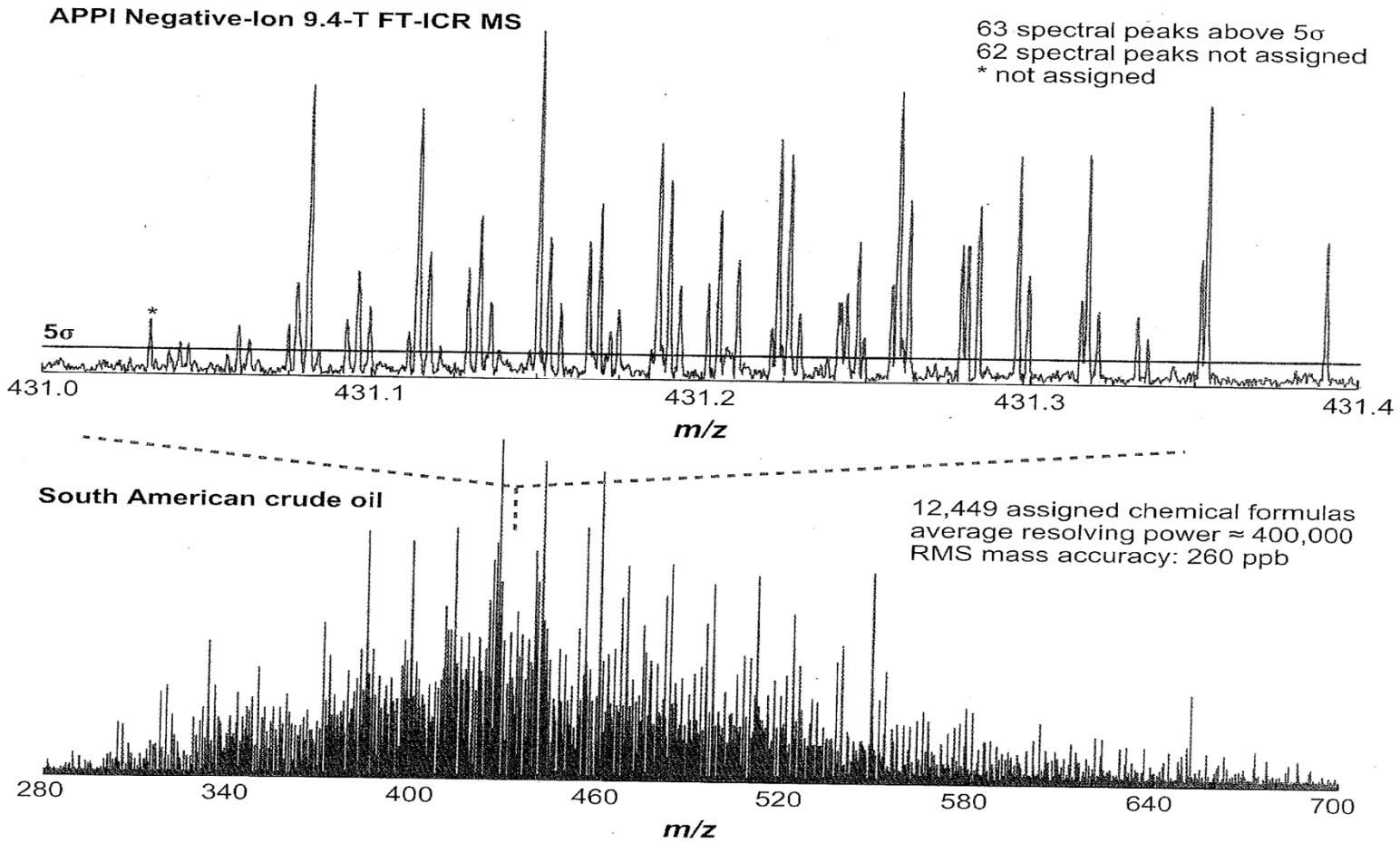
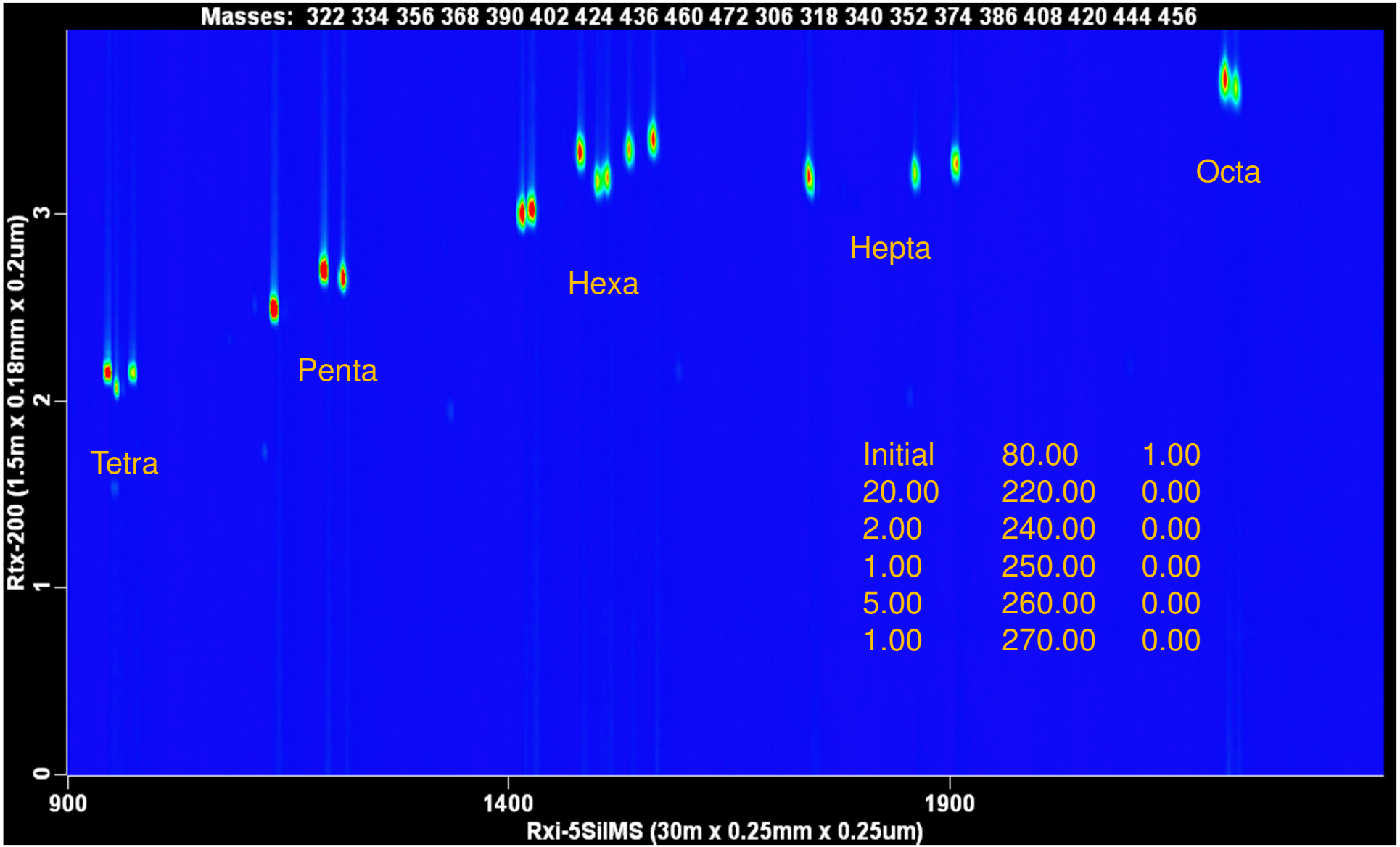


Figure 7

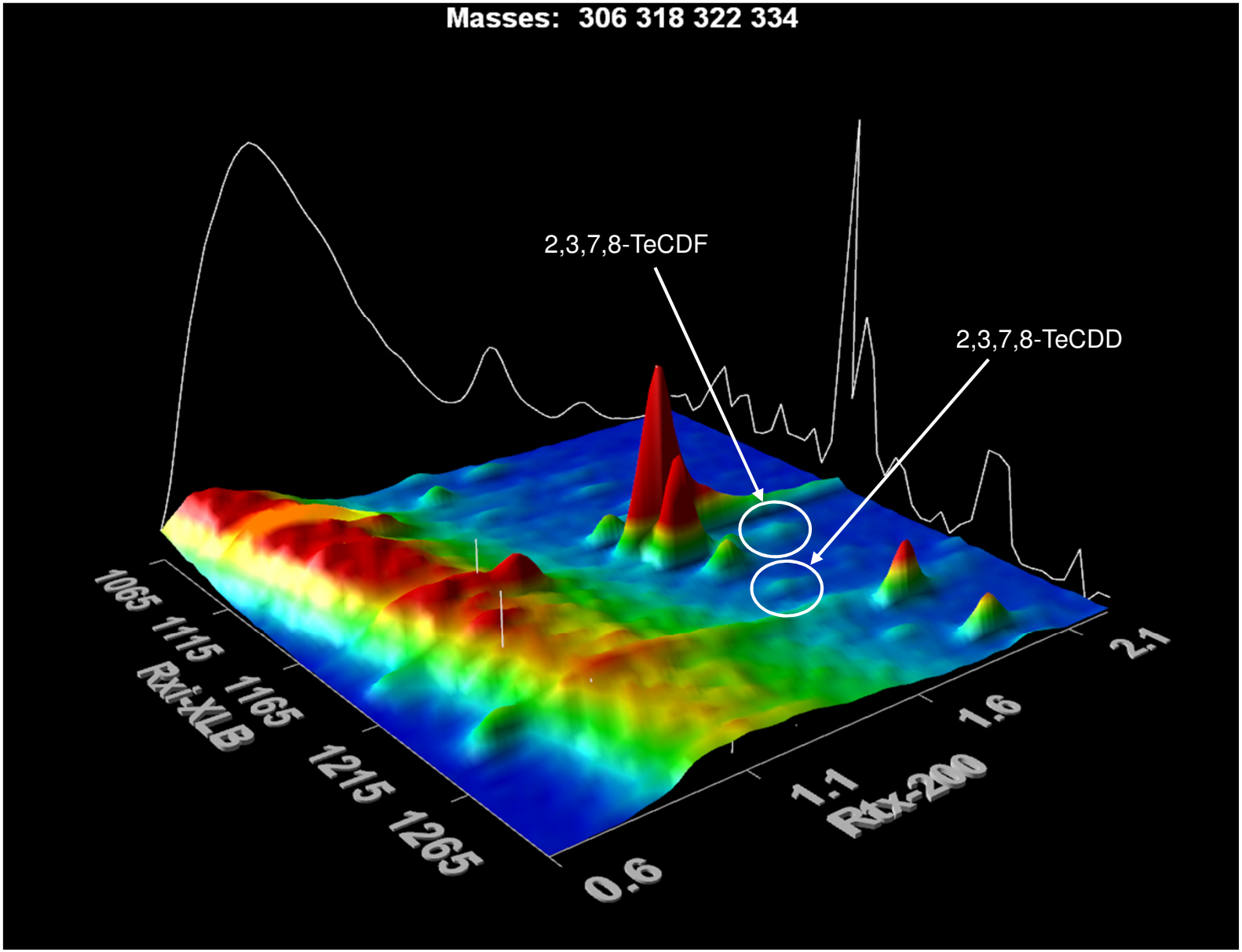
Atmospheric pressure photoionization negative ion 9.4-T Fourier transform–ion cyclotron resonance (FT-ICR) mass spectrum of a South American crude oil, showing the largest total number (and largest number spanning one Dalton) of assigned elemental compositions published to date. Figure adapted with permission from Reference 73.

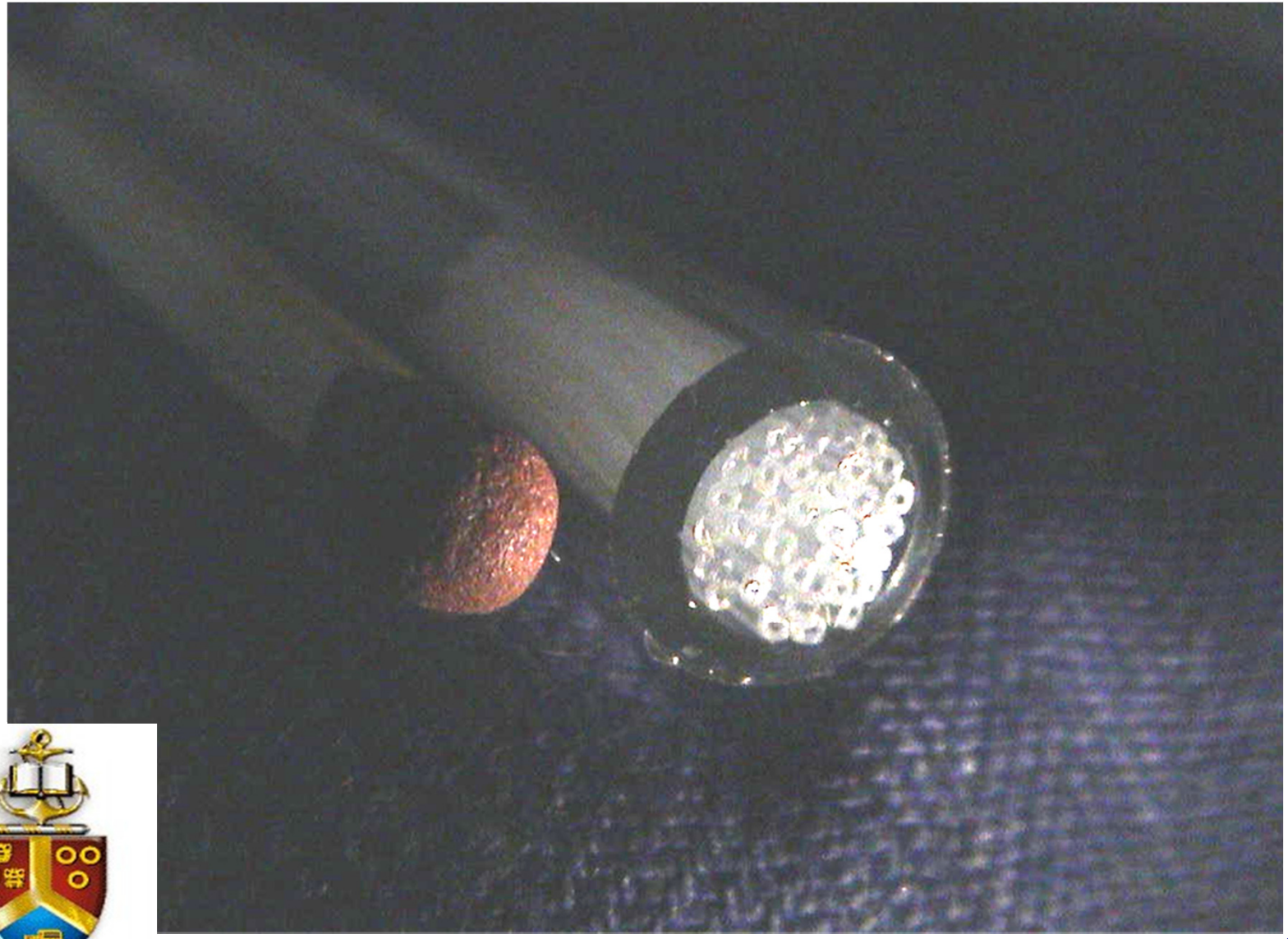
Alan Marshall

Selectivity: Column Combinations



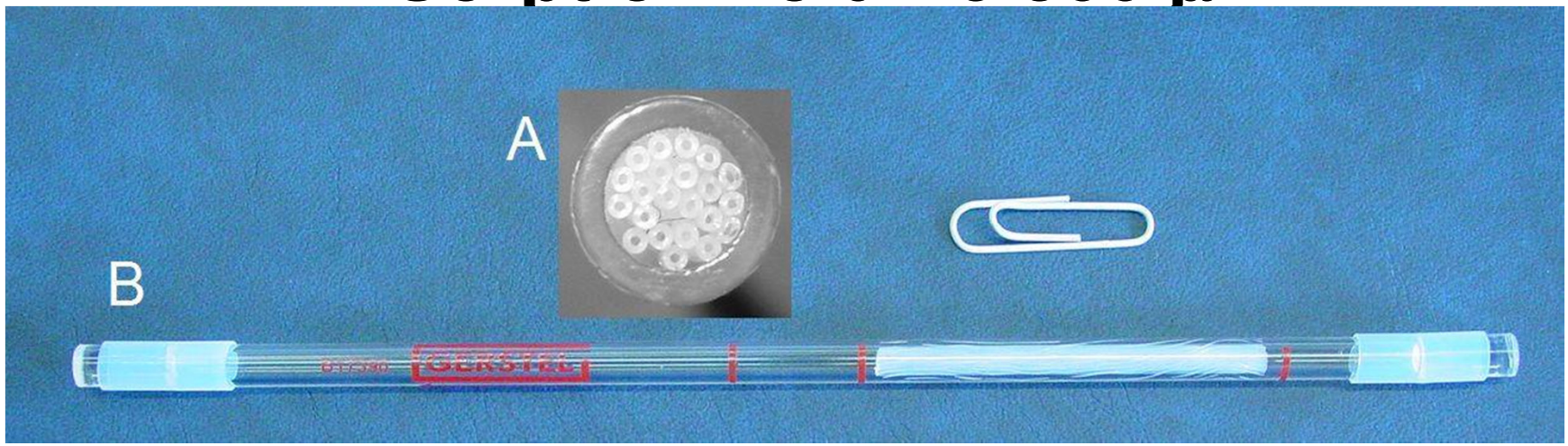
Surface plot - SA sample





Multichannel Silicone (PDMS) Rubber Trap (MCT)

Sorption volume 300 µl



Unique and the heart of a number of our techniques:

1 concentration

2 multi-dimensional chromatography

3 detection

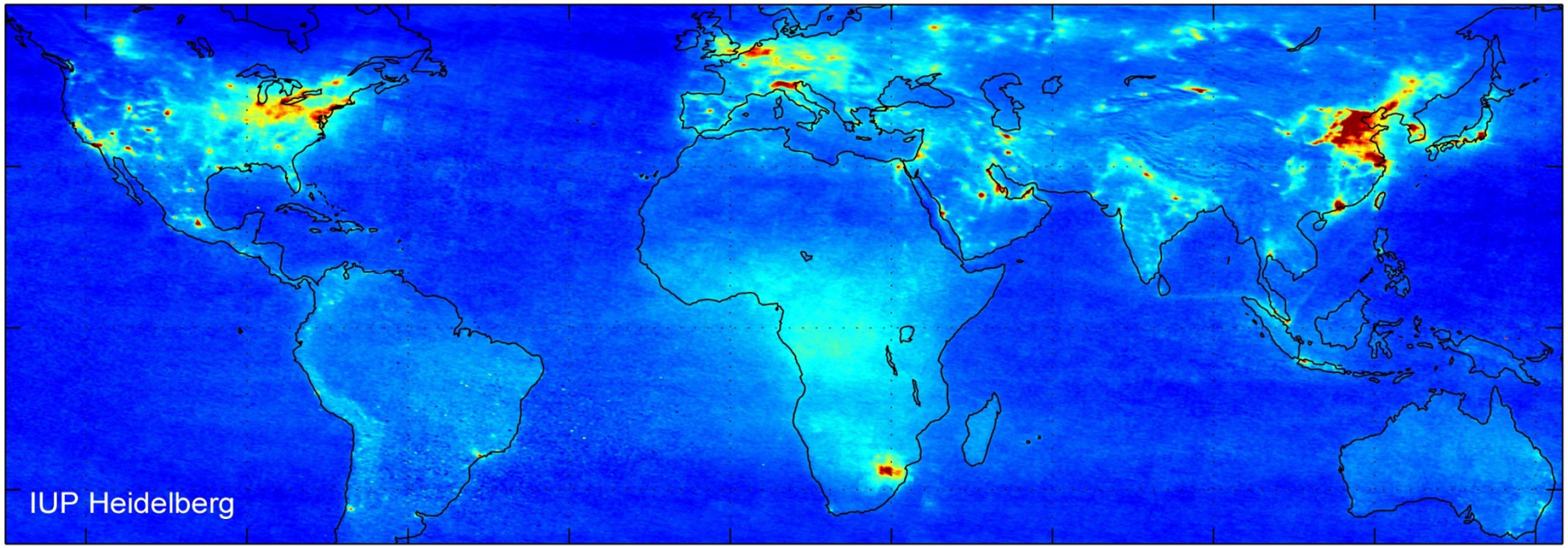
ORTNER, E.K. & *ROHWER, E.R. *Journal of High Resolution Chromatography.* 1996, 18, Jun:339 – 344.

Example 1: Monitoring atmospheric combustion products

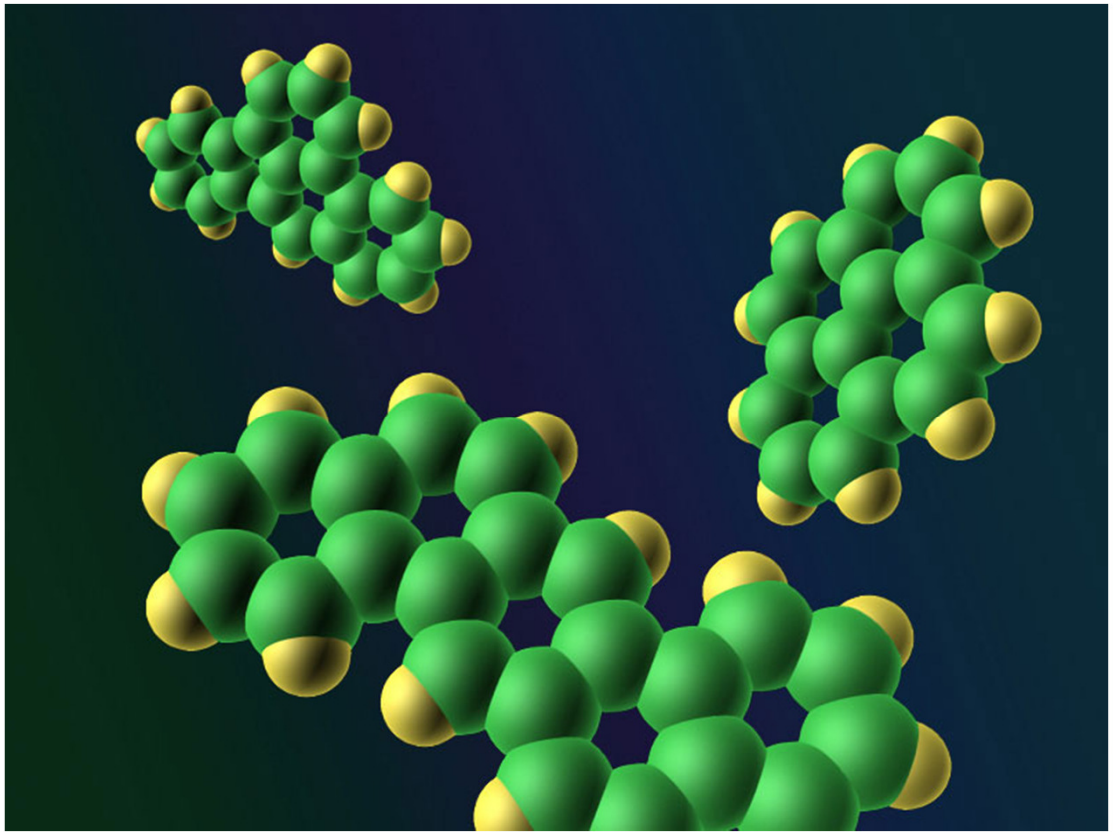
Novelty in our methodology:

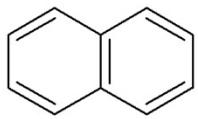
- Screening for impacted areas to reduce numbers of expensive GC-MS analyses
- Laser fluorescence measurements in tube
- Denuder properties of open tubes

NO_2 Pollution

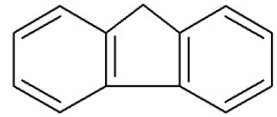


Polycyclic aromatic hydrocarbons (PAHs)

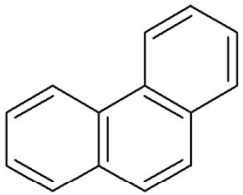




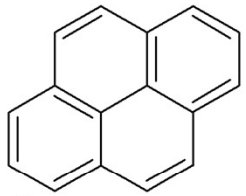
Naphthalene



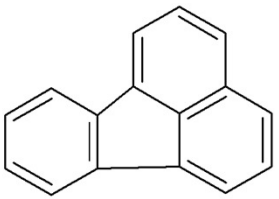
Fluorene



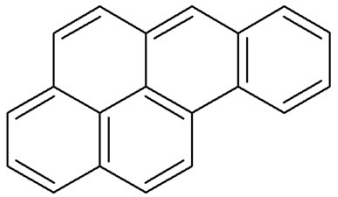
Phenanthrene



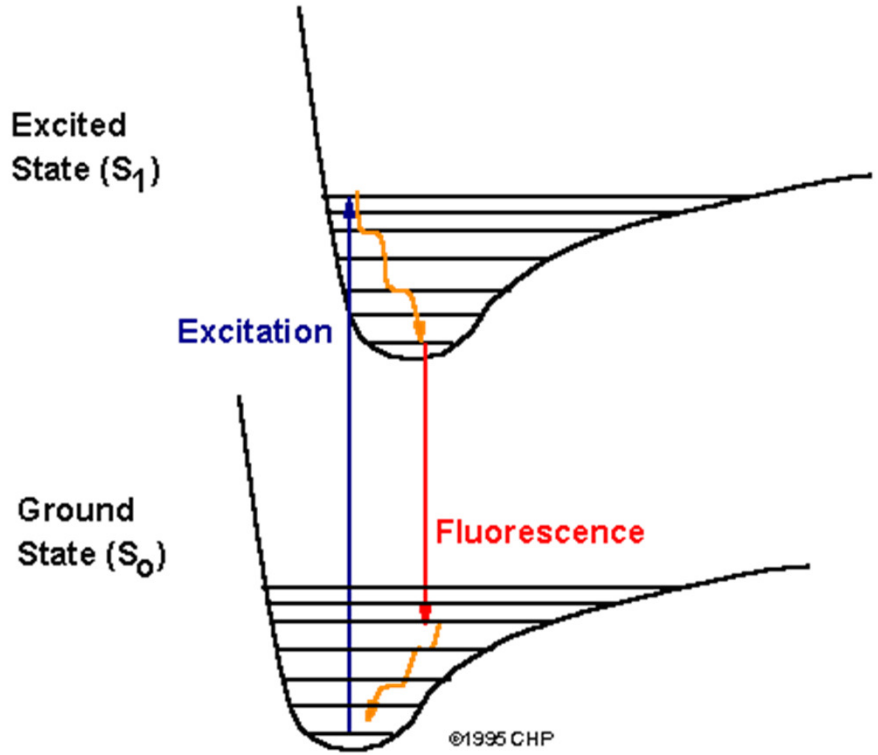
Pyrene



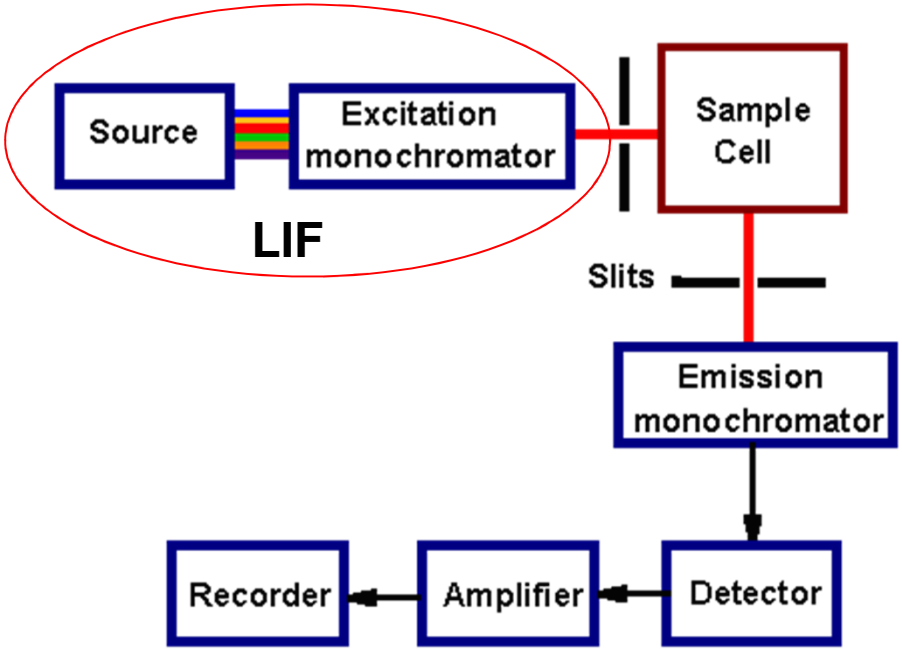
Fluoranthene



Benzo(a)pyrene


Excited
State (S_1)
Excitation
Ground
State (S_o)
Fluorescence
©1995 CHP

Molecular fluorescence spectrometry

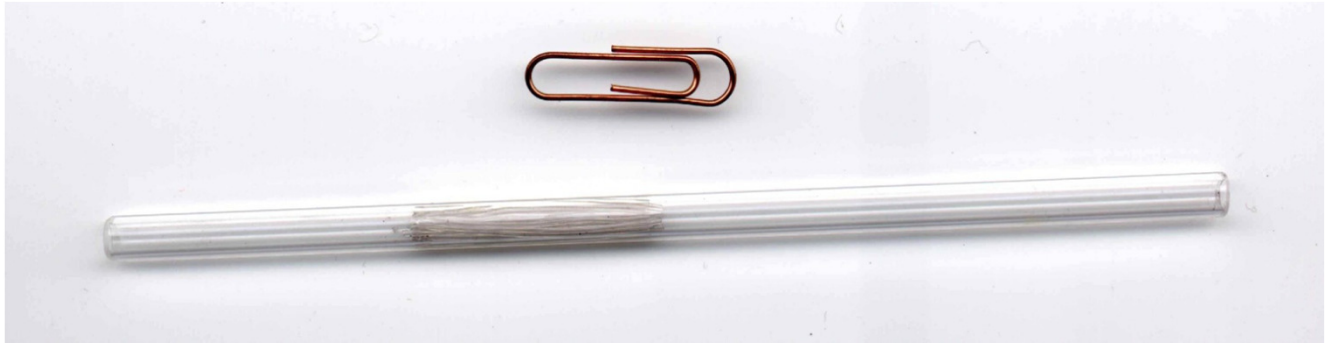


LIF of PAHs

- PAHs have large absorption cross sections and quantum yields (ratio of no. photons emitted to no. photons absorbed thus indicates efficiency of fluorescence process)
- Usually the $\pi \rightarrow \pi^*$ transitions are most probable
- Fluorescence thus used in HPLC detectors for PAHs in solution for many years

PAH	Excitation (nm)	Emission (nm)
Naphthalene	292	323
Phenanthrene	298	364
Fluoranthene	365	462
Pyrene	341	395

Multi-channel silicone rubber sample traps



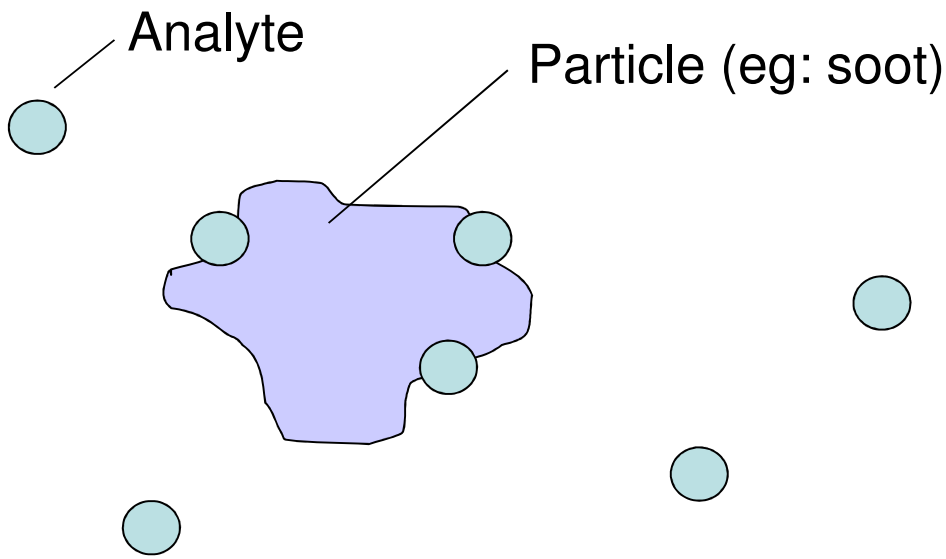
Quartz tube: 3.5 mm i.d.; 160 mm long.
22 PDMS channels, each 0.64 mm o.d. & 0.3 mm i.d.
& 55 mm long

Applications
Sugar cane burn

Human health effects of PAHs

Naphthalene causes haemolytic anaemia and is a possible human carcinogen

Benzo(*a*)pyrene is a suspected human carcinogen



Monitoring particulate and non-particulate air pollutants

Denuder MCT – filter – MCT sampler

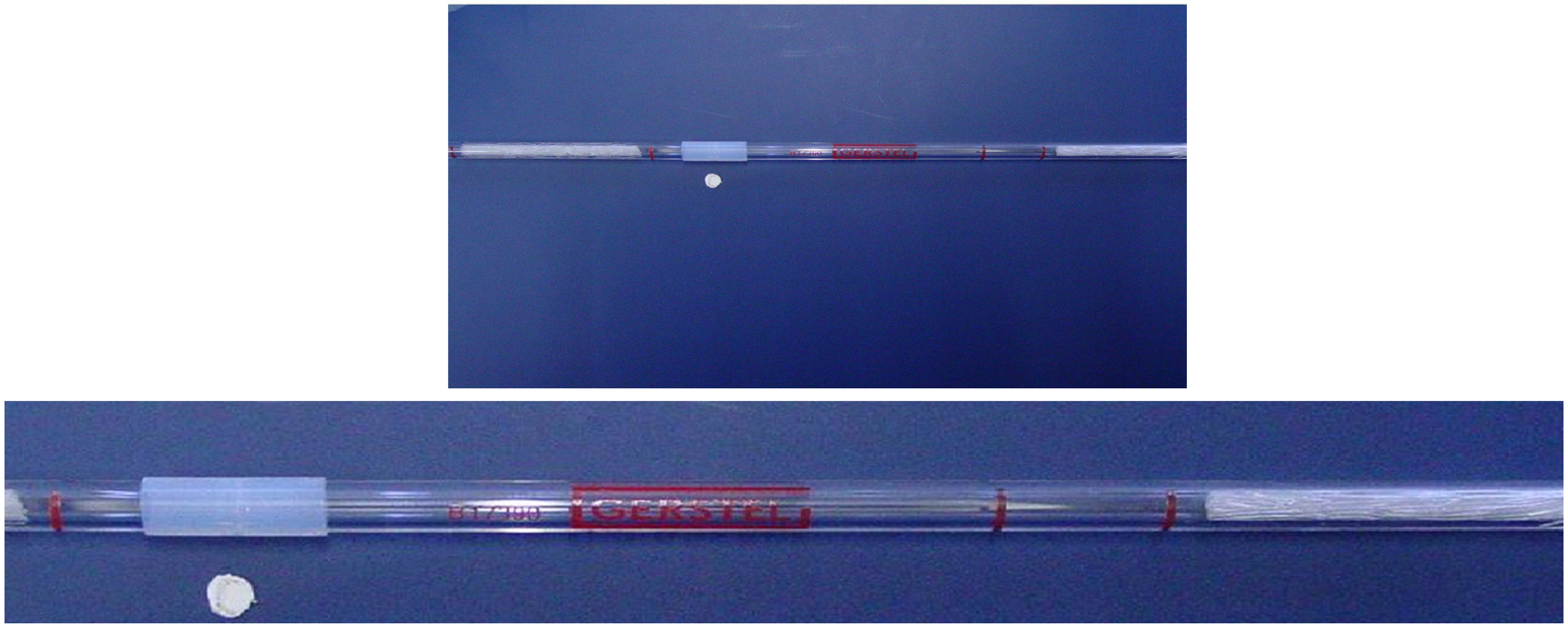
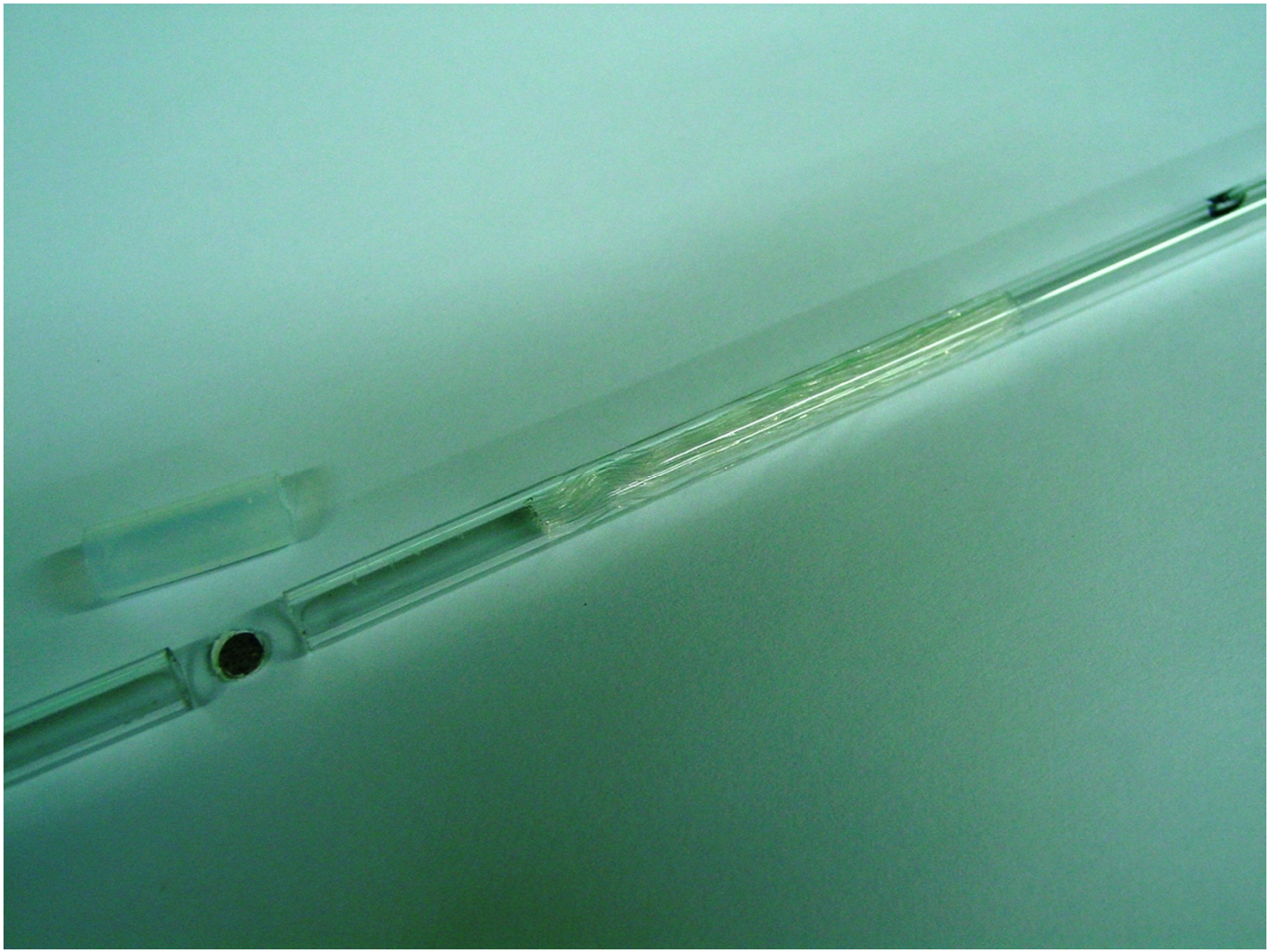


Figure 2. Serially coupled low pressure-drop denuder MCT – quartz micro-fibre filter – MCT system. The MCTs and filter fit a commercial glass desorption tube. The MCTs are connected in series with Tefon (PTFE) tubing.

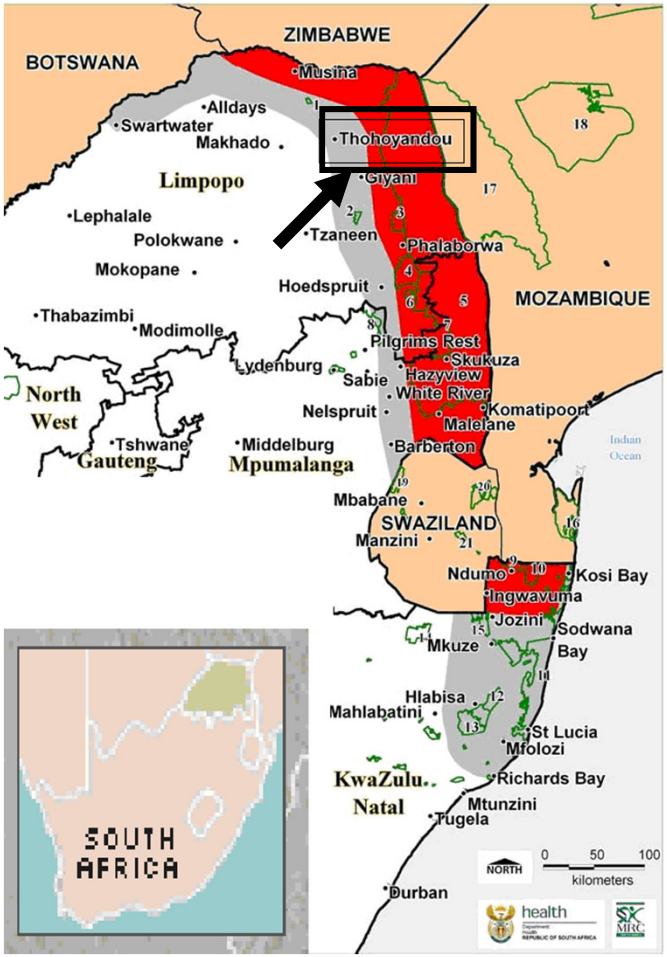
Denuder/filter/denuder after smoke sampling



Example 2: Monitoring atmospheric and soil contamination by DDT

Novelty in our methodology:

- Denuder properties of open tubes allow measurement of exposure to free molecular as well as aerosol bound DDT
- Capture of GC peaks allows re-injection for chiral analysis of o,p DDT and o,p DDD (forensic environmental application)



Study area – Vhembe District, Limpopo Province, South Africa. Red: high malaria risk area. Grey: low malaria risk area.

Persistent organic pollutant: DDT

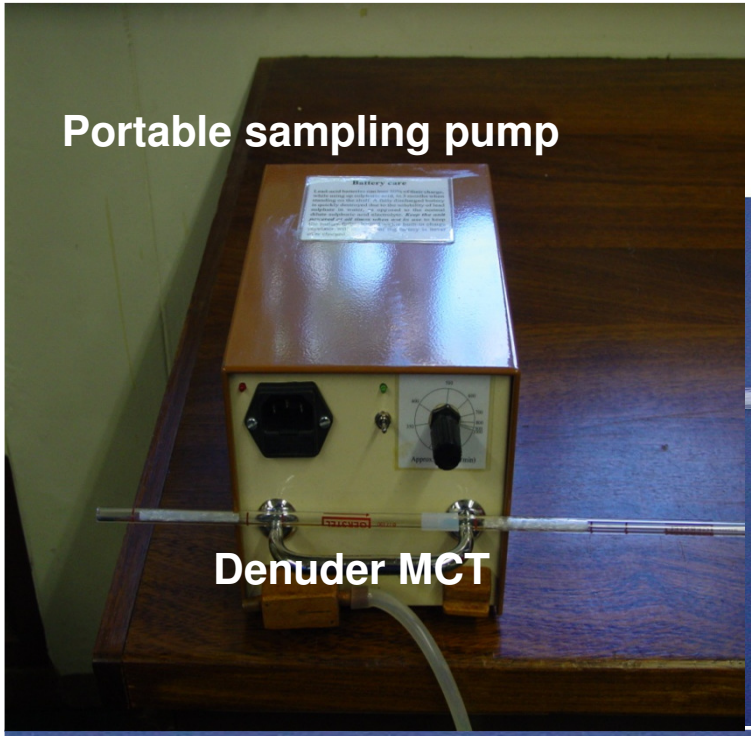
- In rural parts of South Africa the pesticide 1,1,1-trichloro-2,2-bis(4-chlorophenyl)ethane (DDT) is still used for malaria vector control.
- 1 120 cases of malaria reported between July 2009 - January 2010 in Limpopo, South Africa.
- According to the strict international Stockholm (POPs) convention, traditional dwellings are sprayed on the inside with small quantities of technical DDT.

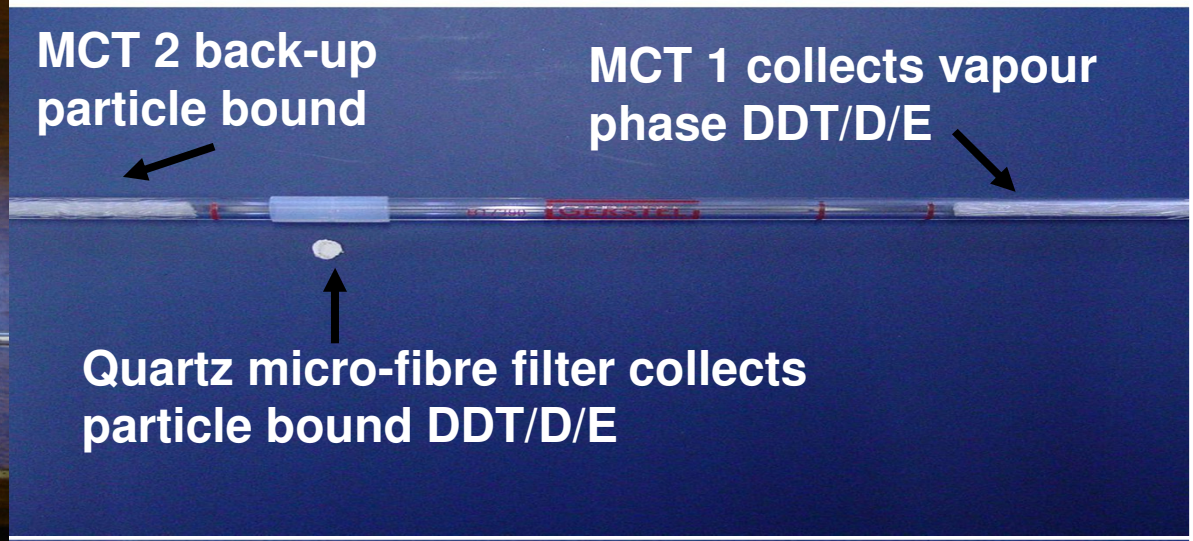
Controlled spraying of huts with DDT

Controlled spraying of huts with DDT

Denuder MCT

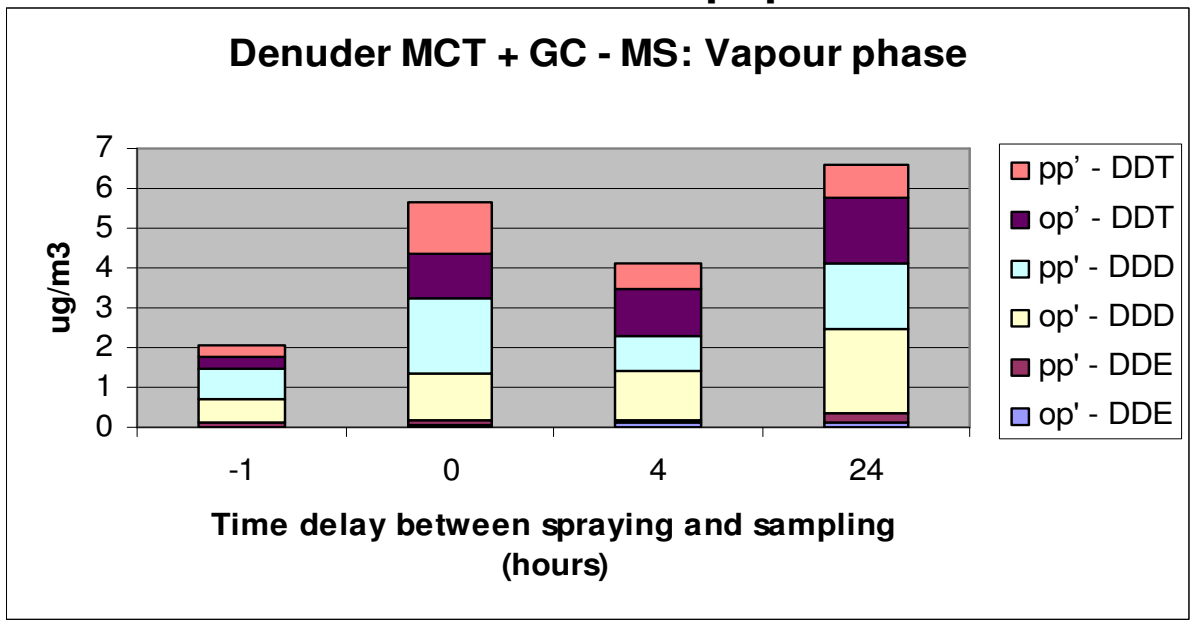
Separate but simultaneous sampling of free molecular and particle bound DDT

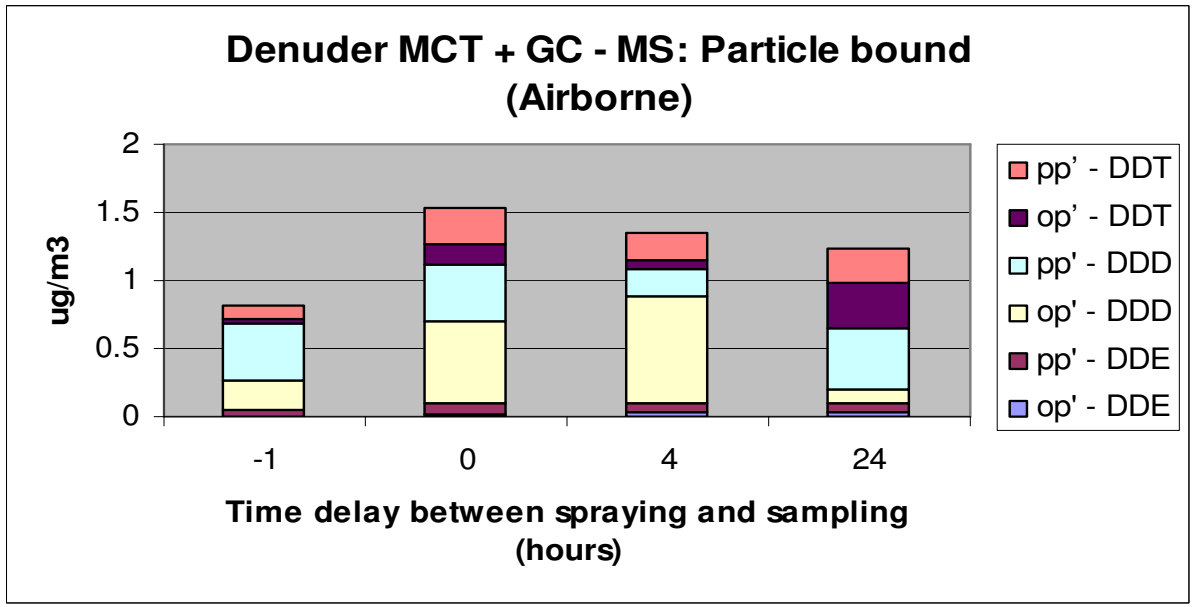


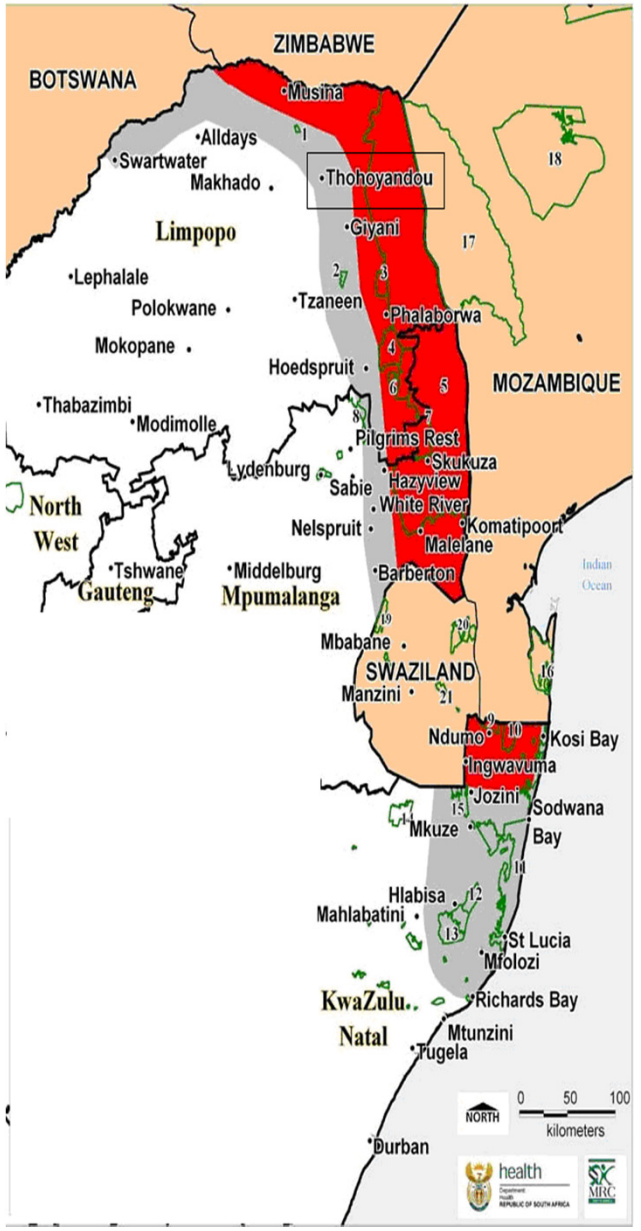


Portable, battery operated, field sampling system.

Indoor Air of Huts in the Limpopo Province







- Technical DDT consists of approximately 65-75% *p,p'*-DDT and 15-25% *o,p'*-DDT.

- *o,p'*-DDT shows enantioselective estrogenecity and biodegradability.

- Thus, it is important to analyse enantiomers of *o,p'*-DDT and its chiral degradation product, *o,p'*-DDD, for both health and environmental-forensic considerations.

Table 1 Structure, nomenclature, molecular formula and weight of the chiral isomers *o,p*'-DDT and *o,p*'- DDD

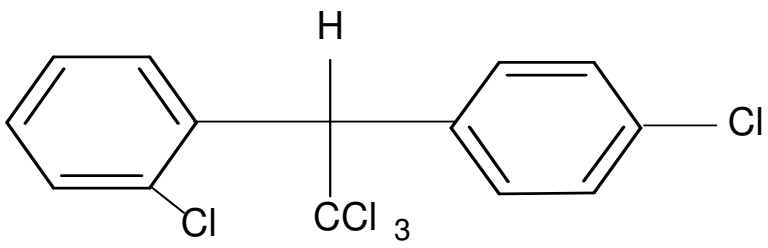
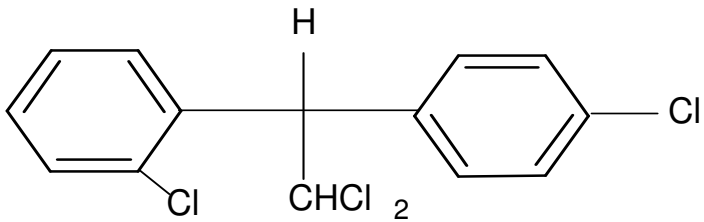
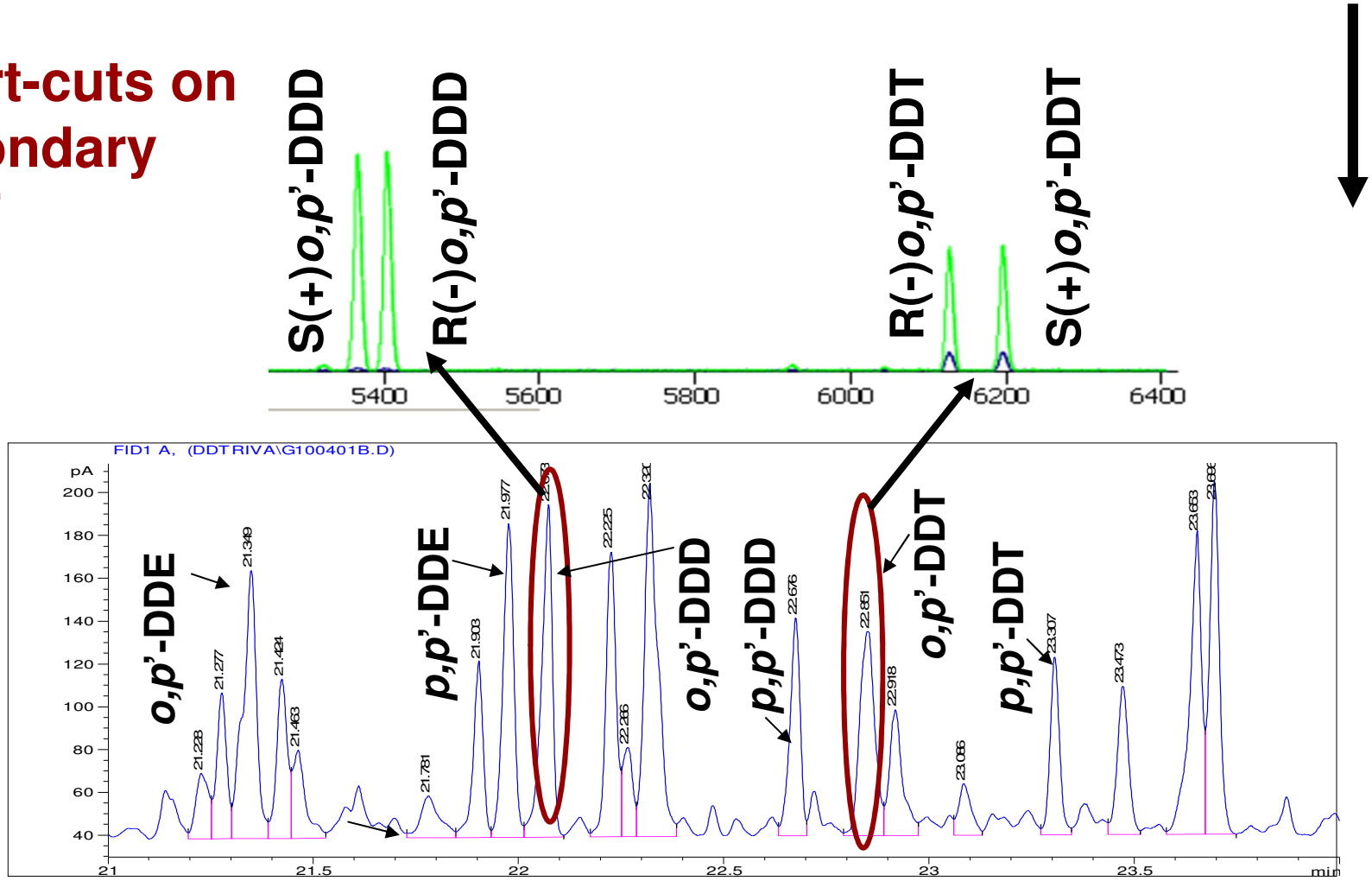
	
_o,p_'- DDT 1,1,1-trichloro-2-(*o*-chlorophenyl)-2-(*p*-chlorophenyl)ethane $C_{14}H_9Cl_5$ 354.49	**_o,p_'- DDD** 1,1-dichloro-2-(*o*-chlorophenyl)-2-(*p*-chlorophenyl)ethane $C_{14}H_{10}Cl_4$ 320.04

Fig. 2. Removed detector top assembly and collector. MCT placed on GC-FID flame tip to recapture single peaks or various fractions [17].

A Heart-cuts on secondary MCT

B Whole sample on primary MCT



[A]Heart-cuts separated on a chiral column (β-cyclodextrin). [B]Non-chiral separation of the corresponding *o,p*'-DDT/D peaks. [A]Enantiomeric order of elution [1].

Example 3: Analysis of environmental trace hydrocarbons of geological origin

Novelty in our methodology:

- Solvent and Artifact-free trace hydrocarbon analysis
- Soil analysis with silicone loops in contact with a few gram of sample (in field or lab)

Sorptive extraction with Multichannel Silicone Rubber (PDMS) Traps (MCTs) and Loops

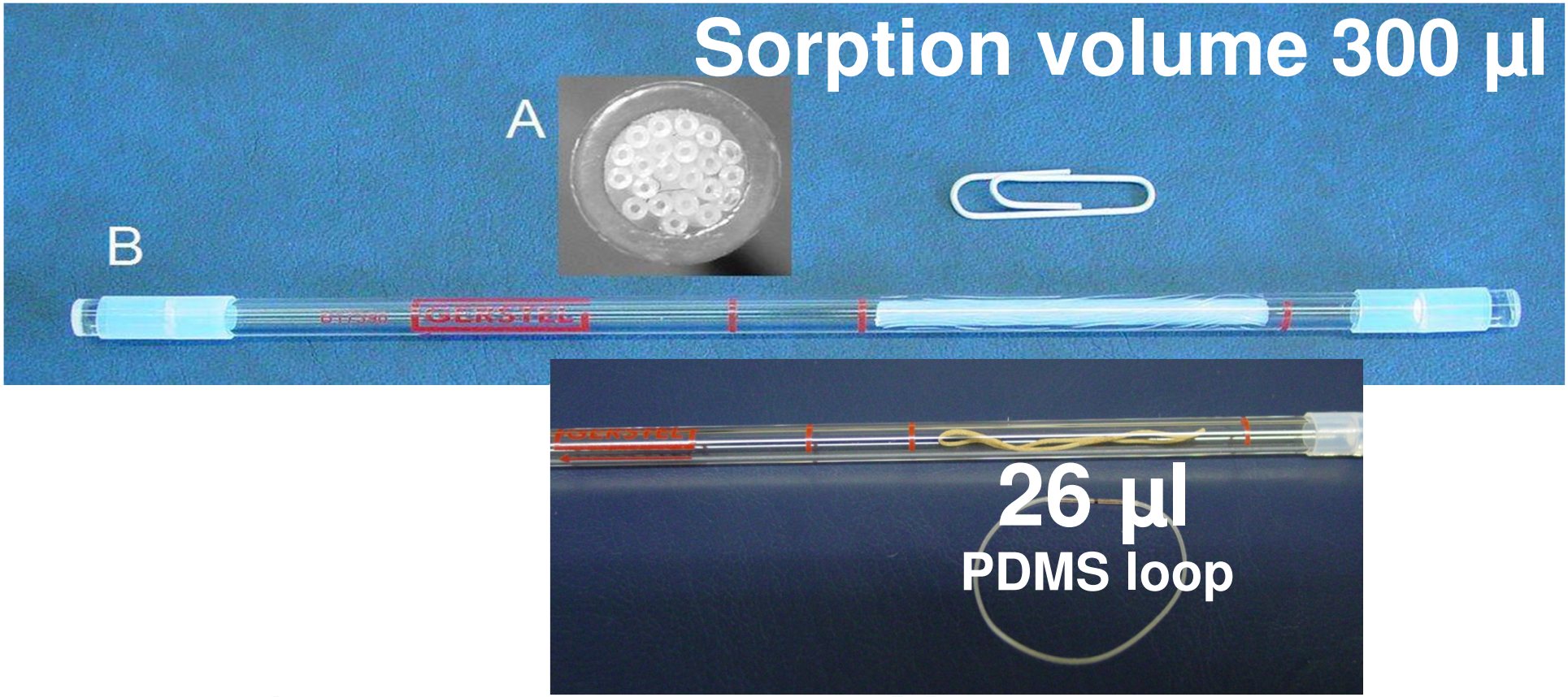
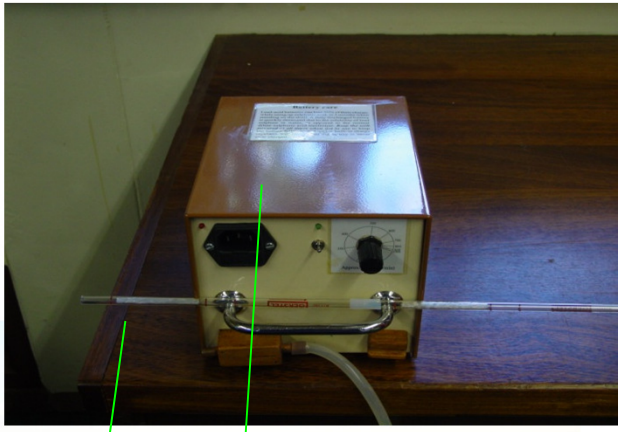


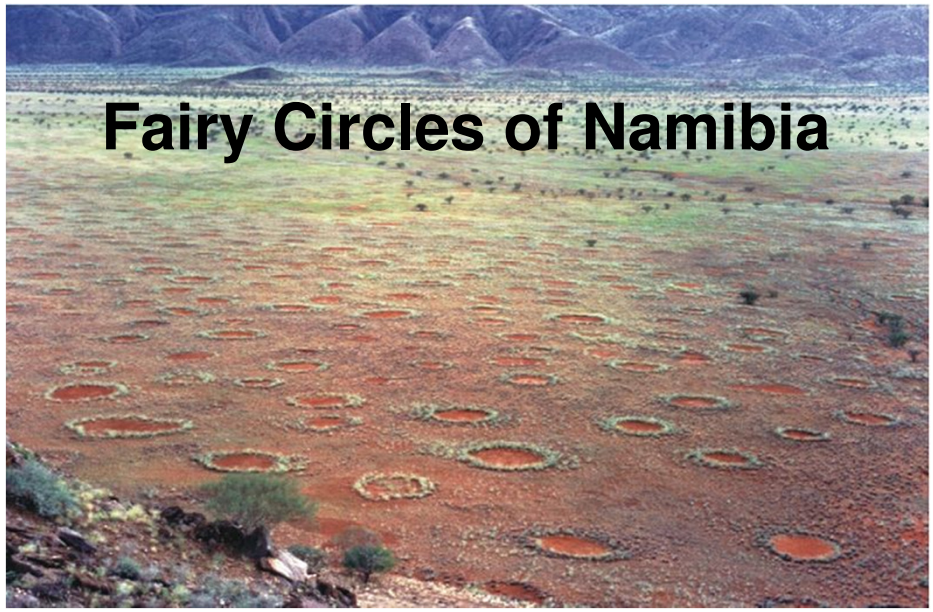
Figure 2. [A]Cross section of a MCT. [B,D]MCT/Loop fits a commercial glass desorption tube.

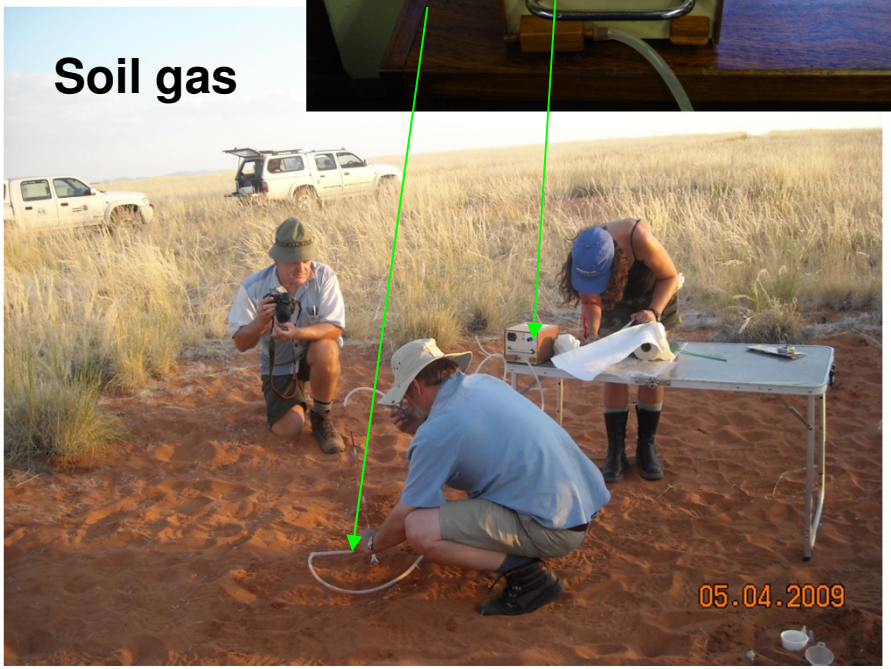
Evidence for a geochemical origin of the mysterious circles in the Pro-Namib desert. **Yvette Naudé, Margaretha van Rooyen and Egmont Rohwer.** ***Journal of Arid Environments, 75(2011) 446-456 .***

"Traditional Himba belief holds that beneath the edge of the Namib Desert, the oldest desert in the world, lies a crack in the earth's crust. A dragon lives there. Whenever he exhales, bubbles of fire rise to the surface, burning the vegetation, causing it to completely vaporise, forming circles."

- Geobotanical manifestation of natural gas microseeps
- Portable, rugged (desert!)
- Sand: PDMS loop for passive extraction







Example 4: Aroma investigations

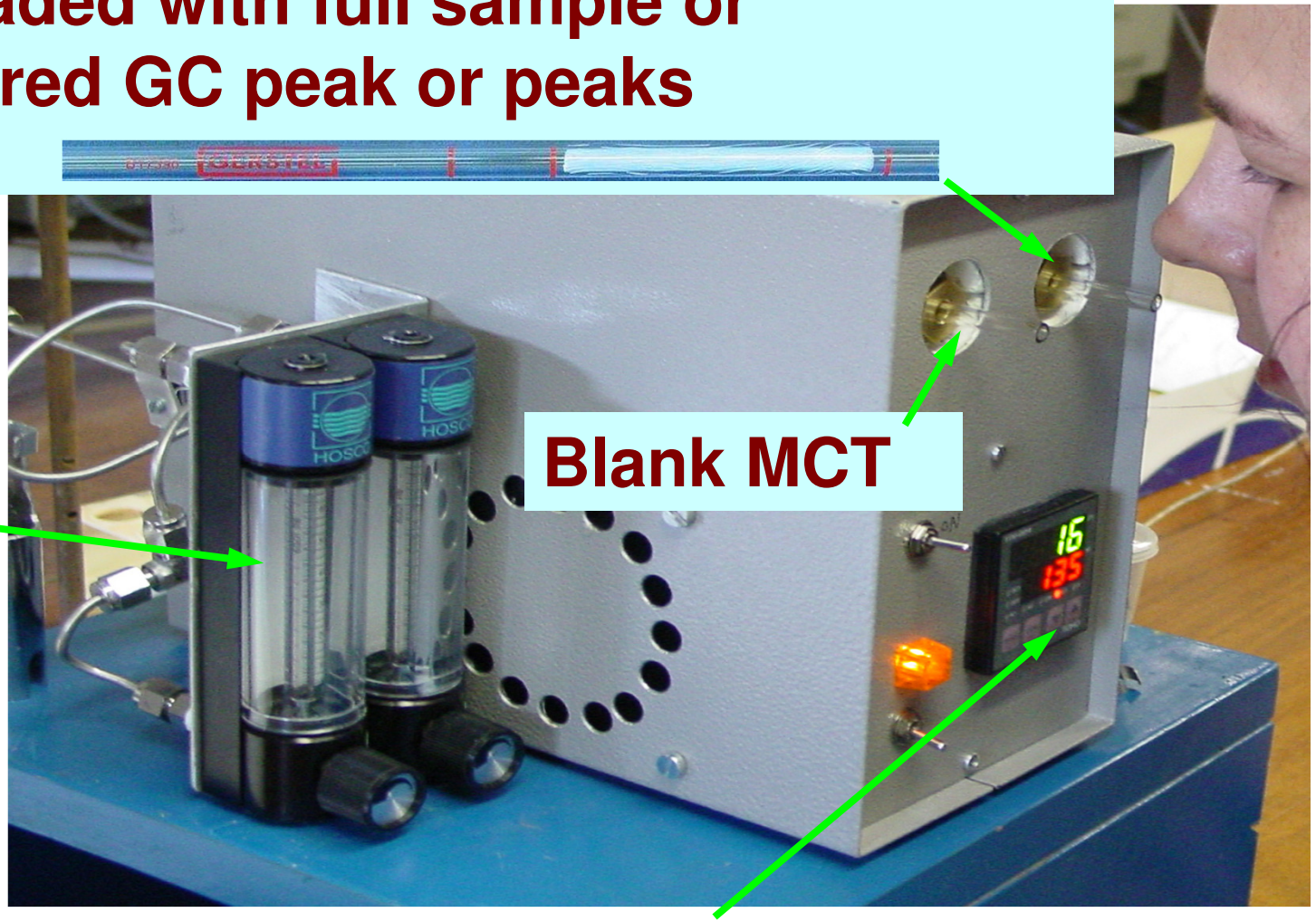
Novelty in our methodology:

- Screening by nose of full trap contents
- GC- fraction or single peak capture for olfactometric assessment (synergism !)
- Re-injection of positive fractions for GC-MS or GCxGCMS identification of components

Fig. 2. Removed detector top assembly and collector. MCT placed on GC-FID flame tip to recapture single peaks or various fractions [17].

Off-line Olfactometry: Slow Release of Aroma or off-odours from MCTs

MCT loaded with full sample or recaptured GC peak or peaks



Synergistic perception of aroma compounds

2-Heptanone

2-Nonanone

Fruity

\+

2-Heptanone

Soapy

\+

2-Nonanone

Sweet

\+

2-Heptanone

Floral

= Blue Cheese

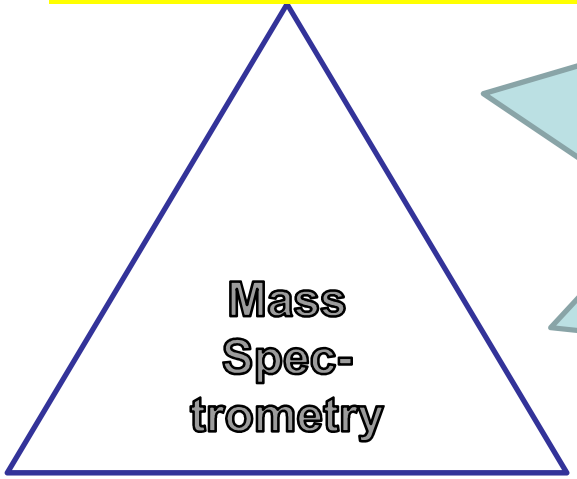
This blue cheese aroma was absent when 2-Heptanone and 2-Nonanone were sniffed individually!

Y. Naudé *et al.* *J. Chromatogr. A* 1216 (2009) 2798–2804.

Exponential growth in sub-discipline: Mass Spectrometry

Electronics
Vacuum technology
Physics
Computers
Lasers
New devices

Motivation:
(i) Sustainable development
(ii) Expanding the technology toolbox ("senses") of chemistry

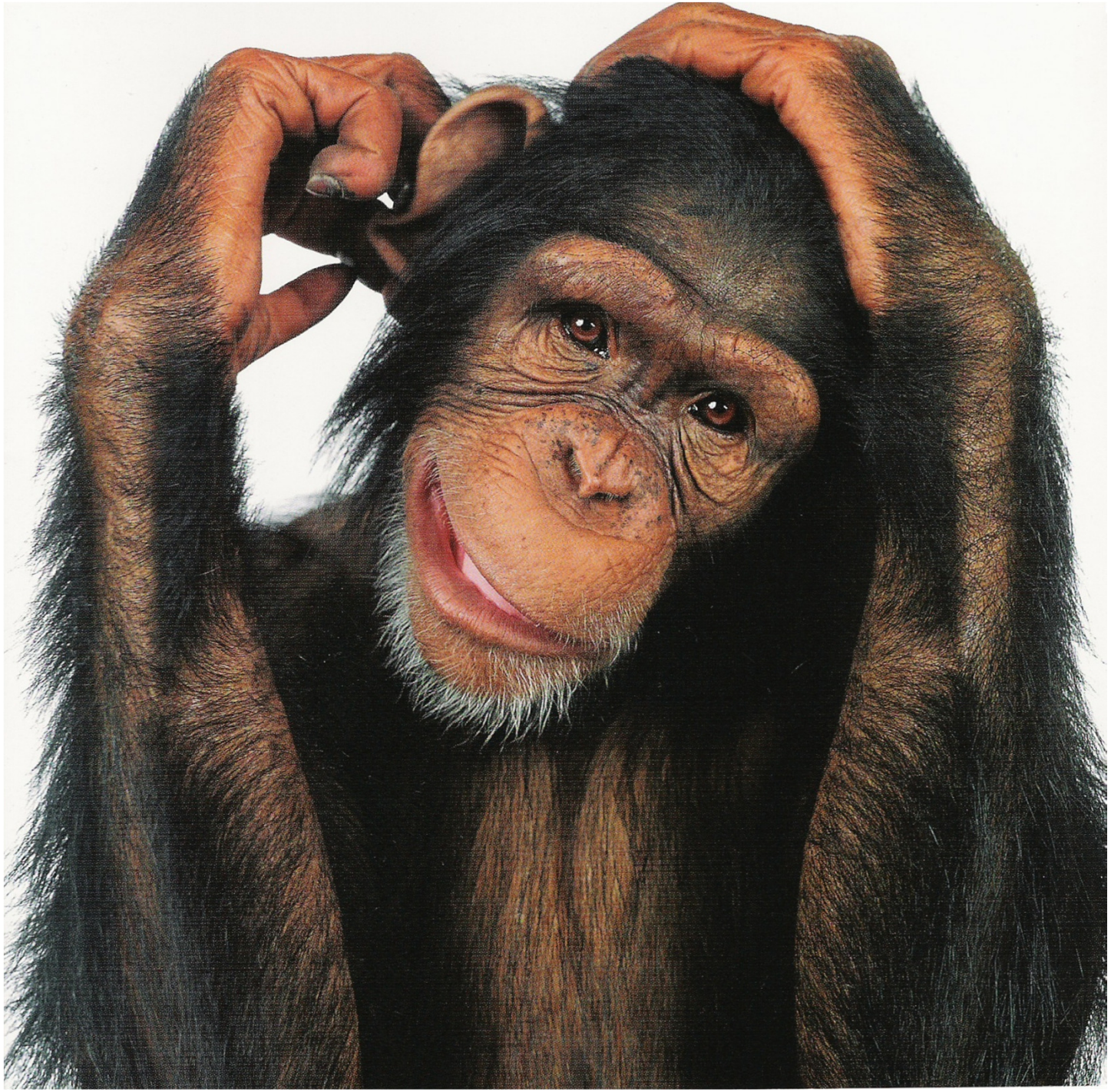


MS Equipment development

Sample Analysis
Analytical information
SERVICE to others

The bigger picture

- Make yourself useful, also do applied work, and you and your very expensive infrastructure will survive! (Nobody finances your personal hobby)
- Academia has a longer term vision and has a responsibility to lead where industry and government cannot (yet). Alliances come later.
- There is synergy between the curiosity driven “blue sky” research and applied science . Both drive your discipline and satisfy your curiosity.
- I discovered the ultimate satisfaction of combining my playful and innovative character with my desire to make a difference.



Thanks to the post graduate students involved in recent work

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- Patricia Forbes
- Jayne de Vos
- Elize Smit
- Marc Bouwer
- Niel Malan
- All former post grad students

Thanks to collaborators involved from other Departments

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• Prof Gretel van Rooyen	Botany
• Prof Mike Wingfield	FABI
• Prof Bernard Slippers	FABI
• Prof Lise Korsten	Plant Pathology
• Prof Elna Buys	Food Science
• Prof Riette de Kock	Food Science
• Prof Riana Bornman	Urology
• Prof Tian de Jager	Urology
• Dr Duncan Cromarty	Pharmacology
• Prof Ralf Zimmermann	Univ Rostock

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- LECO Mr Philip Langenhoven, Dr Peter Gorst-Allman, Mr Alex Whaley
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- National Laser Centre (NLC)

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- Dr Fanie van der Walt
- Dr Jack Cochran
- Mr David Masemula
- Nico van Vuuren
- Leon Engelbrecht
- Naomi Steenkamp

Structure of lecture

- Introduction
- Historical perspective
- Personal research experience, with emphasis on recent years
- Vision for the Department

Vision 2025 of the University

"to be a leading research-intensive university in Africa, recognised for its quality, relevance and impact, and also for developing people, creating knowledge and making a difference locally and globally."

President Barack Obama (Nobel laureate)

- at the US National Academy of Science (NAS) annual meeting (27 April 2009), referring to present economic problems:

"At such a difficult moment, there are those who say we cannot afford to invest in science, that support for research is somehow a luxury at moments defined by necessities. I fundamentally disagree. Science is more essential for our prosperity, our security, our health, our environment, and our quality of life than it has ever been before."

- C&EN; Jan 2010

"The nation that out-educates us today is going to out-compete us tomorrow. To continue to cede our leadership in education is to cede our position in the world."

The **True Size** of **Africa**

A small contribution in the fight against rampant *Immappancy*, by **Kai Krause**

Graphic layout for visualization only (some countries are cut and rotated)
But the conclusions are very accurate: refer to table below for exact data

COUNTRY	AREA x 1000 km²
China	9.597
USA	9.629
India	3.287
Mexico	1.964
Peru	1.285
France	633
Spain	506
Papua New Guinea	462
Sweden	441
Japan	378
Germany	357
Norway	324
Italy	301
New Zealand	270
United Kingdom	243
Nepal	147
Bangladesh	144
Greece	132
TOTAL	**30.102**
AFRICA	**30.221**

In addition to the well known social issues of *illiteracy* and *innumeracy*, there also should be such a concept as "*immappancy*", meaning *insufficient geographical knowledge*.

A survey with random American schoolkids let them guess the population and land area of their country. Not entirely unexpected, but still rather unsettling, the majority chose *"1-2 billion"* and *"largest in the world"*, respectively.

Even with Asian and European college students, geographical estimates were often off by factors of *2-3*. This is partly due to the highly distorted nature of the predominantly used mapping projections (such as *Mercator*).

A particularly extreme example is the worldwide misjudgement of the true size of *Africa*. This single image tries to embody the massive scale, which is larger than the *USA, China, India, Japan* and *all of Europe..... combined!*

Top 100 Countries

Area in square kilometers, Percentage of World Total
Sources: Britannica, Wikipedia, Almanac 2010

		AREA km²	%
1	Russia	17.098.242	11,50
2	Canada	9.984.670	6,70
3	China	9.596.961	6,40
4	United States	9.629.091	6,40
5	Brazil	8.514.877	5,70
6	Australia	7.692.024	5,20
7	India	3.287.263	2,30
8	Argentina	2.780.400	2,00
9	Kazakhstan	2.724.900	1,80
10	Sudan	2.505.813	1,70
11	Algeria	2.381.741	1,60
12	Congo	2.344.858	1,60
13	Greenland	2.166.086	1,50
14	Saudi Arabia	2.149.690	1,40
15	Mexico	1.964.375	1,30
16	Indonesia	1.860.360	1,30
17	Libya	1.759.540	1,20
18	Iran	1.628.750	1,10
19	Mongolia	1.564.100	1,10
20	Peru	1.285.216	0,86
21	Chad	1.284.000	0,86
22	Niger	1.267.000	0,85
23	Angola	1.246.700	0,85
24	Mali	1.240.192	0,83
25	South Africa	1.221.037	0,82
26	Colombia	1.141.748	0,76
27	Ethiopia	1.104.300	0,74
28	Bolivia	1.098.581	0,74
29	Mauritania	1.025.520	0,69
30	Egypt	1.002.000	0,67
31	Tanzania	945.087	0,63
32	Nigeria	923.768	0,62
33	Venezuela	912.050	0,61
34	Namibia	824.116	0,55
35	Mozambique	801.590	0,54
36	Pakistan	796.095	0,53
37	Turkey	783.562	0,53
38	Chile	756.102	0,51
39	Zambia	752.612	0,51
40	Myanmar	676.578	0,45
41	Afghanistan	652.090	0,44
42	Somalia	637.657	0,43
43	France	632.834	0,43
44	C. African Rep	622.984	0,42
45	Ukraine	603.500	0,41
46	Madagascar	587.041	0,39
47	Botswana	582.000	0,39
48	Kenya	580.367	0,39
49	Yemen	527.968	0,35
50	Thailand	513.120	0,34
51	Spain	505.992	0,34
52	Turkmenistan	488.100	0,33
53	Cameroon	475.442	0,32
54	Papua New Guinea	462.840	0,31
55	Uzbekistan	447.400	0,30
56	Morocco	446.550	0,30
57	Sweden	441.370	0,30
58	Iraq	438.317	0,29
59	Paraguay	406.752	0,27
60	Zimbabwe	390.757	0,26
61	Japan	377.930	0,25
62	Germany	357.114	0,24
63	Rep o.t. Congo	342.000	0,23
64	Finland	338.419	0,23
65	Vietnam	331.212	0,22
66	Malaysia	330.803	0,22
67	Norway	323.802	0,22
68	Côte d'Ivoire	322.463	0,22
69	Poland	312.685	0,21
70	Oman	309.500	0,21
71	Italy	301.336	0,20
72	Philippines	300.000	0,20
73	Burkina Faso	274.222	0,18
74	New Zealand	270.467	0,18
75	Gabon	267.668	0,18
76	Western Sahara	266.000	0,18
77	Ecuador	256.369	0,20
78	Guinea	245.857	0,17
79	United Kingdom	242.900	0,16
80	Uganda	241.038	0,16
81	Ghana	238.539	0,16
82	Romania	238.391	0,16
83	Laos	236.800	0,16
84	Guyana	214.969	0,14
85	Belarus	207.600	0,14
86	Kyrgyzstan	199.951	0,13
87	Senegal	196.722	0,13
88	Syria	185.180	0,12
89	Cambodia	181.035	0,12
90	Uruguay	176.215	0,12
91	Suriname	163.820	0,11
92	Tunisia	163.610	0,11
93	Nepal	147.181	0,10
94	Bangladesh	143.998	0,10
95	Tajikistan	143.100	0,10
96	Greece	131.957	0,09
97	Nicaragua	130.373	0,09
98	North Korea	120.538	0,08
99	Malawi	118.484	0,08
100	Eritrea	117.600	0,08
	TOP 100 TOTAL	132.632.524	89,34

Department of Chemistry research focus areas:

- **Separation Science** (Prof E Rohwer, Dr T Laurens, Dr P Forbes, Dr S Bauermeister, Ms A Botha.)
- **Synthesis and Applications in Organometallic Chemistry** (Prof S Lotz, Dr M Landman, Dr D Bezuidenhout)
- **Synthesis of Biologically-active Compounds** (Prof R Vleggaar Dr L Pilcher, Dr N October, Dr M Nkwelo)
- **Materials and computational chemistry** (Prof P van Rooyen Dr. M Rademeyer, Dr E van der Merwe, Dr J Pretorius, Extr. Prof Casper Schutte)
- **Electrochemistry** (Prof. I. Cukrowski, Extr. Prof K Ozoemena (CSIR))
- **Chemical Education** (Prof. M. Potgieter)
- **Forensic Toxicology** (Dr T Laurens)

New overarching themes of local relevance, to synergistically strengthen the traditional disciplines in Chemistry

- Molecular diagnostic and therapeutic techniques (NECSA, Health sciences, Petlabs …)

- Computer modeling and synthesis of catalysts used for renewable fuels production (IBM, Johnson Matthey, …)

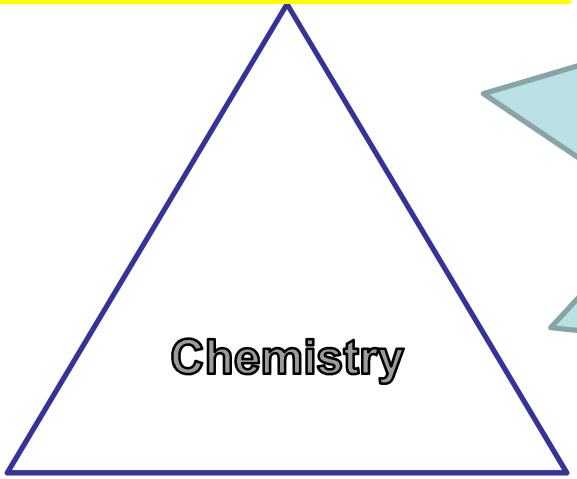
Cost of facilities/ sub-disciplines

- Capital cost/replacement cost
- Running cost, maintenance
- Repair costs
- Skilled, dedicated scientists and operators

All in an environment ("intellectual home") where the sub-discipline is mastered and taught

Exponential growth in the discipline: Chemistry

Analytical technology (facilities) “Toolbox”
MS, NMR, Xray Diff…
Computers



Motivation:
Curiosity/Aesthetics
Quality of life
Power/control

Chemical theory (models)

Application to real problems.
Experiment (reality check)

Evolutionary survival of expensive experimental disciplines in a developing world can only be achieved symbiotically, with a vigilant adaptation to needs

- We, our discipline and our facilities cannot achieve critical mass without reaching out to other fields of science
- We want to make alliances with other UP departments, industry and government to chase our dreams and serve theirs
- We are thankful to have been identified as a base discipline department in need of special help
- We have big dreams and need lots of help to upgrade the facilities we host for all researchers at UP

Anton Rupert, ex-staff member of the Chemistry Department

"He who does not believe in miracles is not a realist"

aan studente by Tukkies (1987):

"Streef nie daarna om bloot suksesvol te wees nie, maar probeer mense van waarde wees. Die suksesvolle man haal dikwels meer uit die lewe as wat hy terugplaas. Die man van waarde, daarenteen, gee meer as wat hy ontvang."

Thanks

- Ms Ria Swart
- All other Colleagues from Chemistry

- Prof Willem Engelbrecht (US)
- Dr Daan Kemp (UCOR/ NECSA)
- Prof Piet van Berge (RAU/ UJ)
- Prof Victor Pretorius

Thanks for planned Departmental collaboration

- Prof Debra Meyer (Biochemistry)
- Prof Philip de Vaal (Chemical Engineering)
- Prof Oppel Greef (Pharmacology)
- Prof Mike Wingfield (FABI)
- Prof Chris Theron (Physics)
- Prof Elna Buys (Food Science)
- Prof Walter Focke (Materials Institute)
- Prof Philip Crouse (SARCHI)
- Prof Ncholu Manyala (SARCHI)
- Prof Innocent Pikirayi (Anthropology & Archeology)
- Prof Fanus Venter (Microbiology and Plant Pathology)
- Prof Hannes Rautenbach (Department of Geography, Geoinformatics and Meteorology)
- *And all other Departments yet to join in….*

Prof Wiseman Nkuhlu - Chancellor UP, at the occasion of our centenary celebration, 2008:

"As we celebrate the achievements of the past, we must think about our stewardship going forward: If we conduct ourselves with integrity, diligence, competence and a deep commitment to serve South Africa, we will build an institution that will last: an institution that will make a unique contribution to the socioeconomic advancement of our country. However, if we allow ourselves to be engulfed by mediocrity and populism, the edifice that has been bequeathed to us will collapse in our own hands to the detriment of the whole country "

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