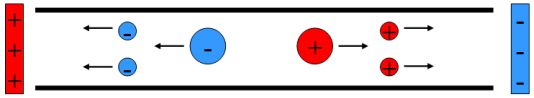
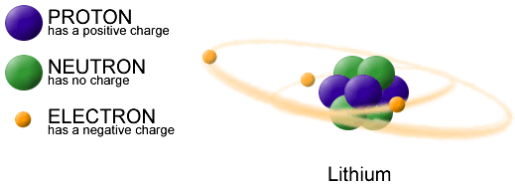
ThermoFisher SCIENTIFIC

Capillary electrophoresis

focusing on chiral separation



Mass spectrometry



MS, GC-MS, LC-MS

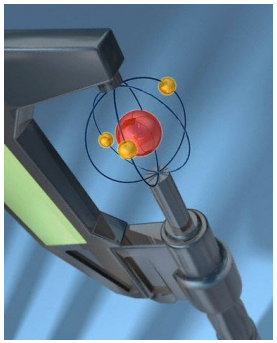
Lukáš Plaček

1. General terms in analytical chemistry (10´; 1 question)

2. Capillary electrophoresis (35´; 2 questions)

3. Mass spectrometry

- In general (25´; 2 questions)
- GC-MS (10´; 1 question)
- HPLC-MS (10´; 1 question)

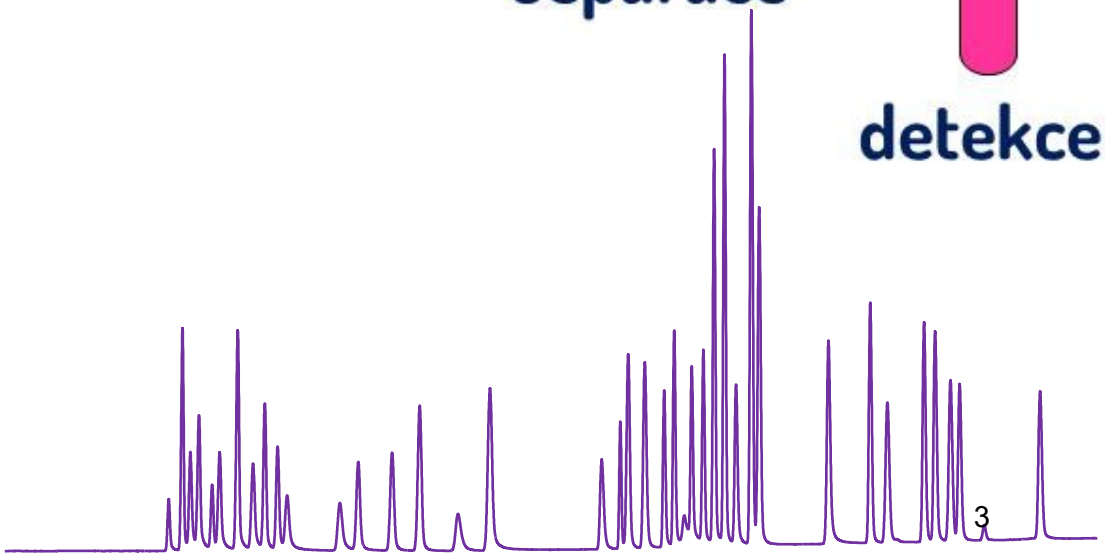


nástřik

separace

detekce

čas



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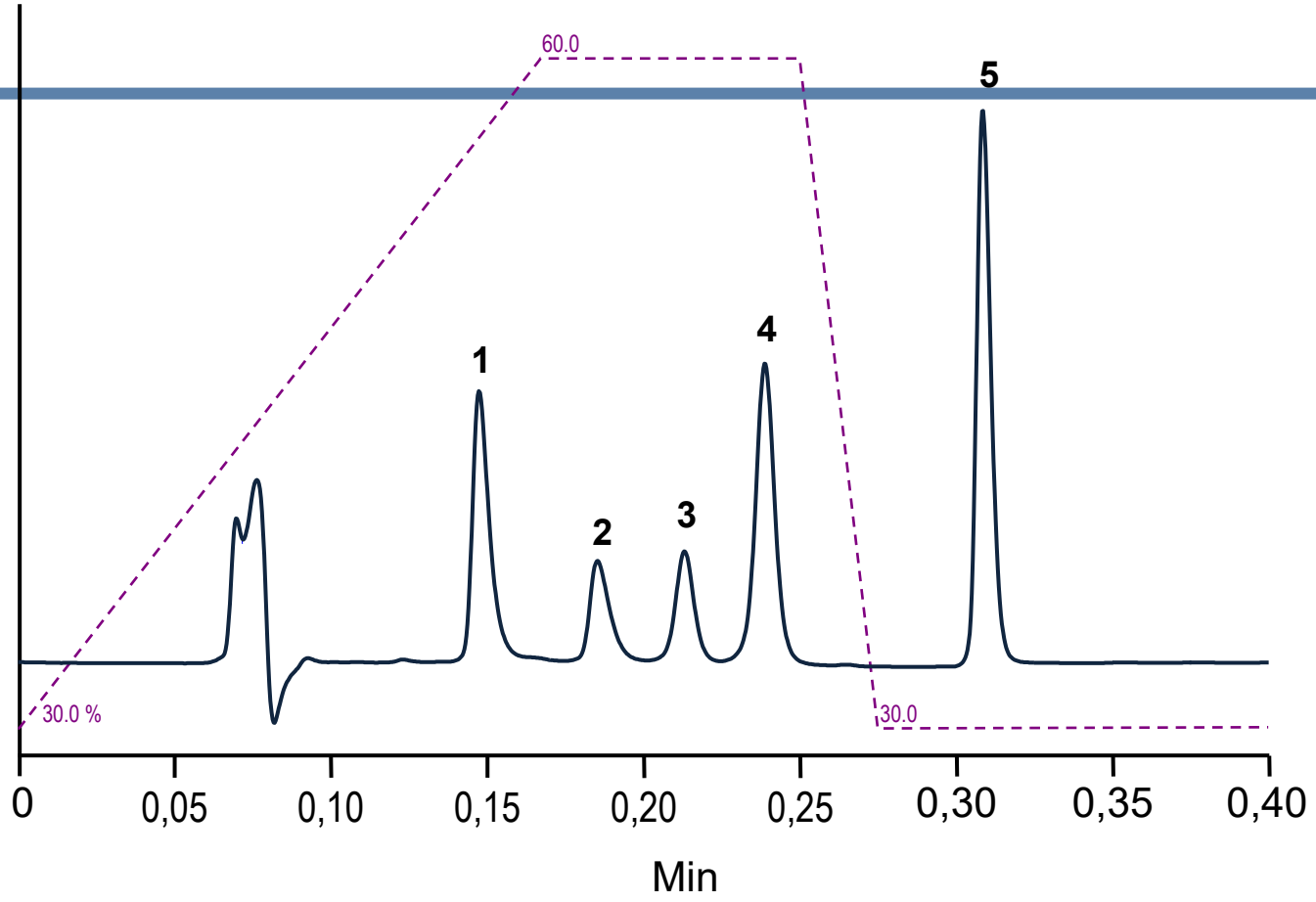
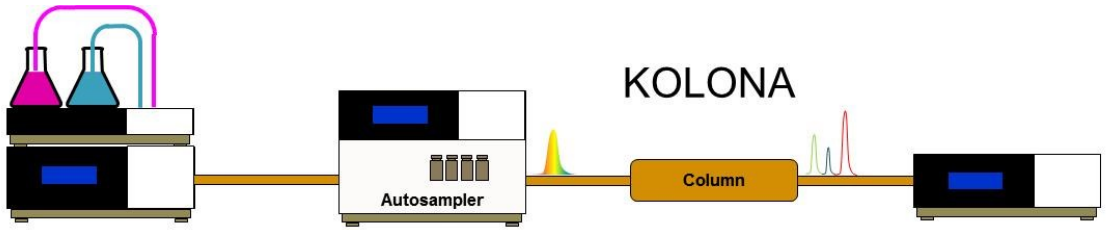
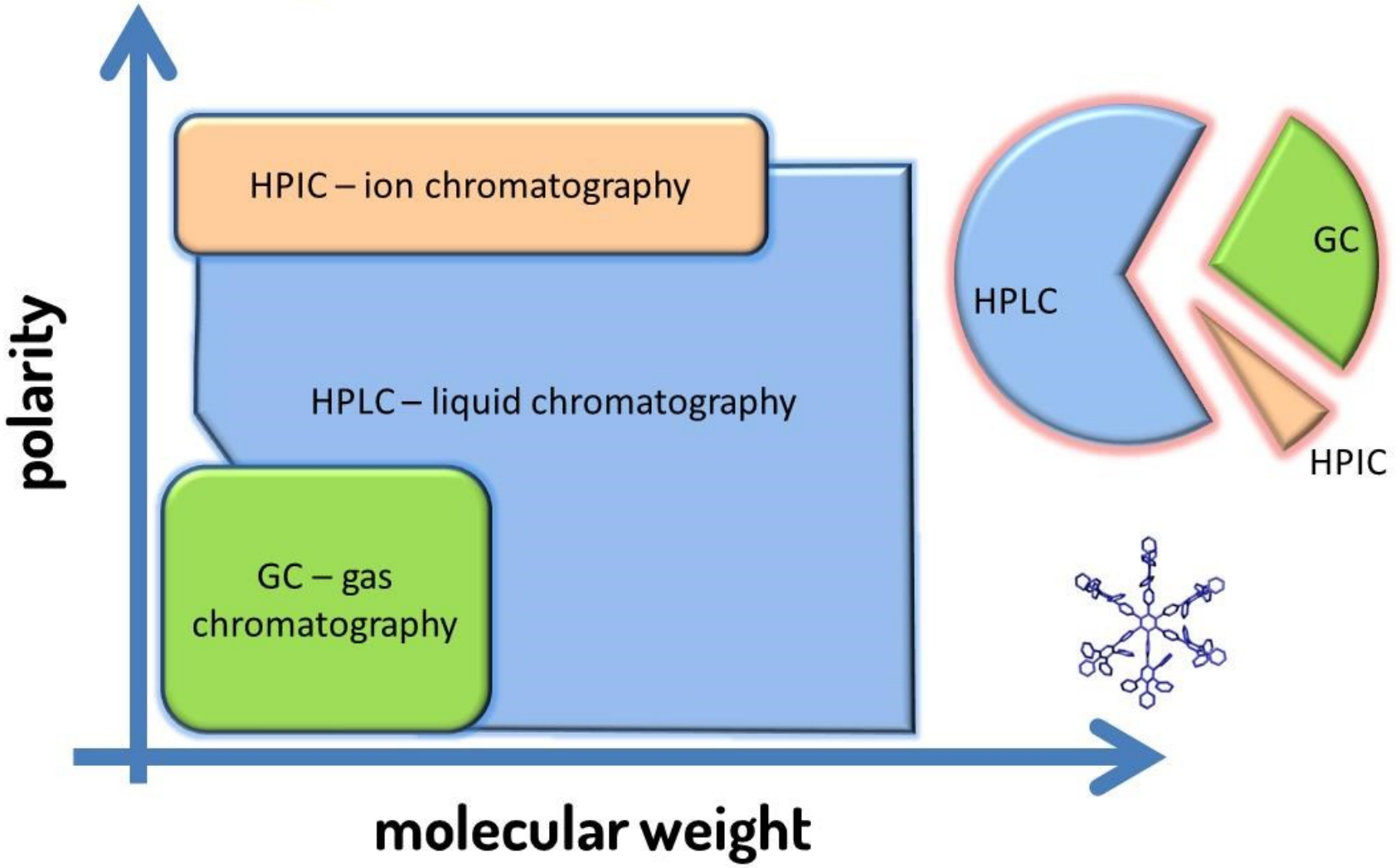




PUMPA AUTOSAMPLER DETEKTOR

ANALYTICAL SEPARATION



ThermoFisher SCIENTIFIC

GENERAL TERMS
IN ANALYTICAL CHEMISTRY

1. **General terms** – Qualitative vs. Quantitative analysis
2. Calibration curve, sensitivity of method
3. Noise, limit of detection, limit of quantitation
4. Accuracy/precision, repeatibility/reproducibility

Terms

Sample, analyte

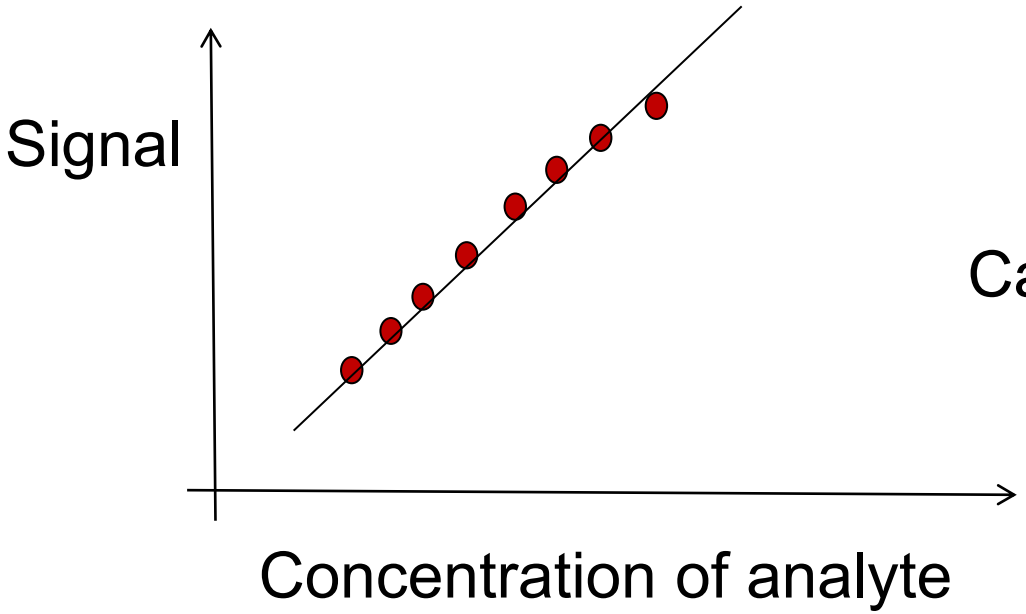
QUALITATIVE
(what?)

- identification of unknown sample
- identification of flammables
- identification of umpurities in Paralen

QUANTITATIVE
(how much/many?)

- determination of Cd in milk
- determination of pervintine in blood
- determination of Hg in hair

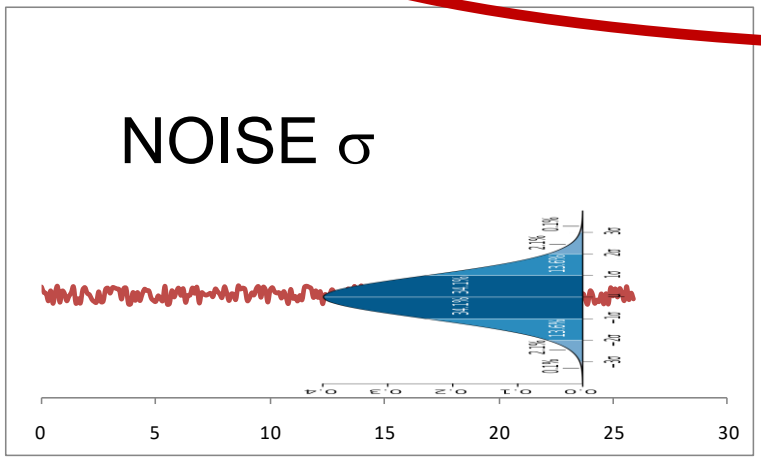
Sensitivity

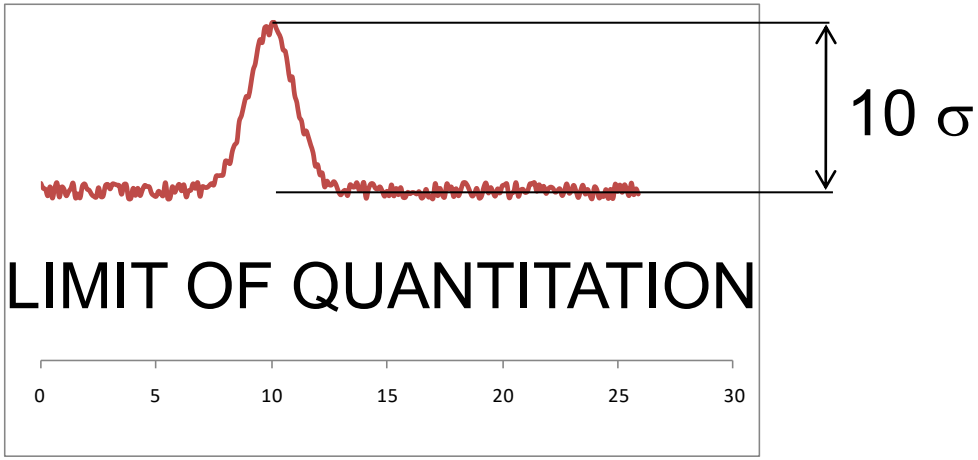


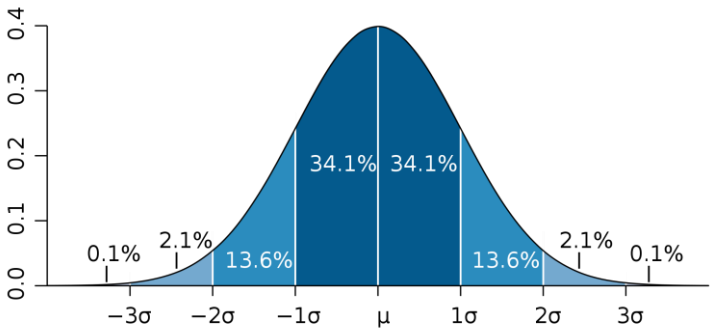
Calibration curve

Sensitivity = slope of calibration curve

LOD, LOQ

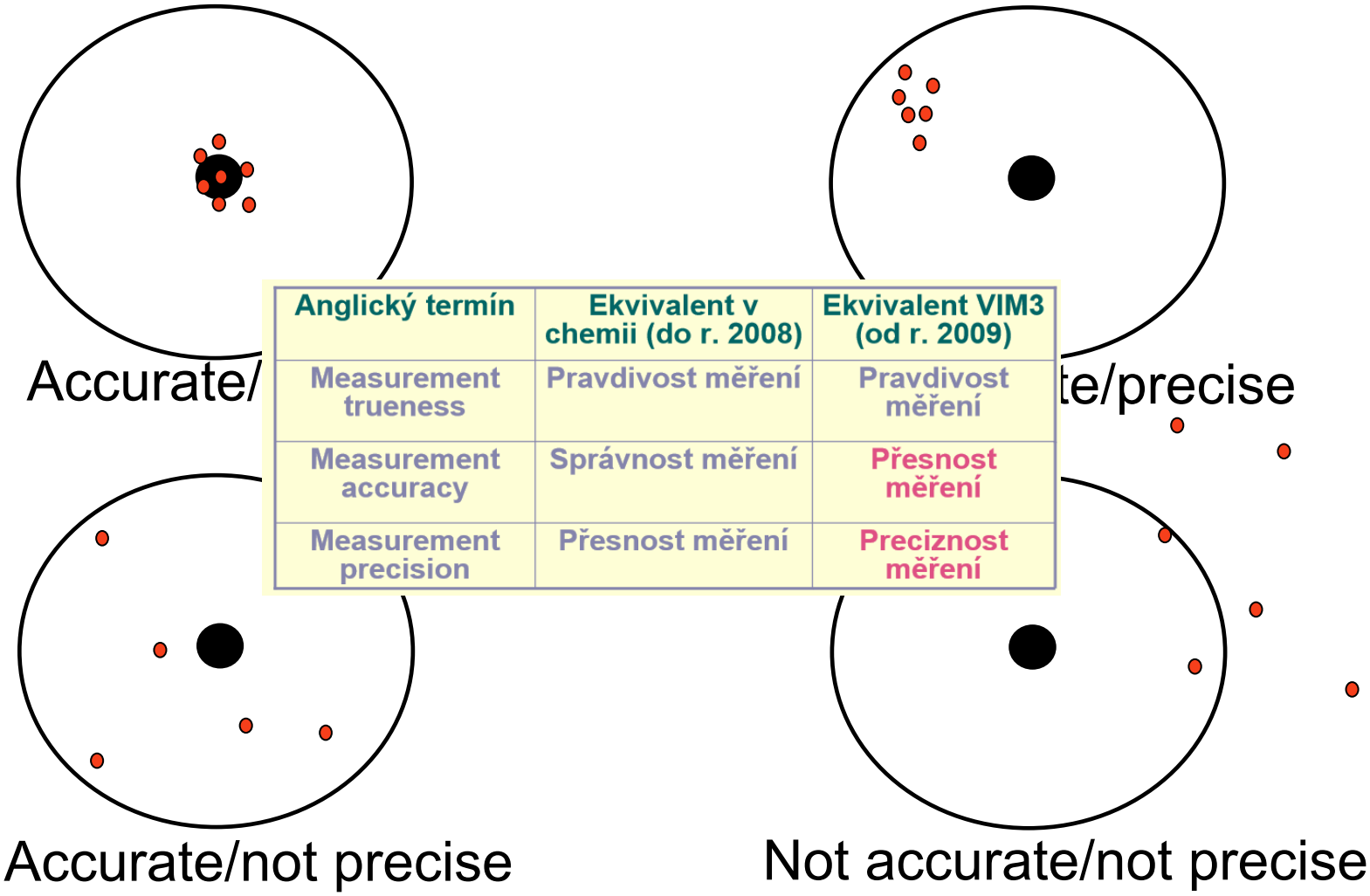






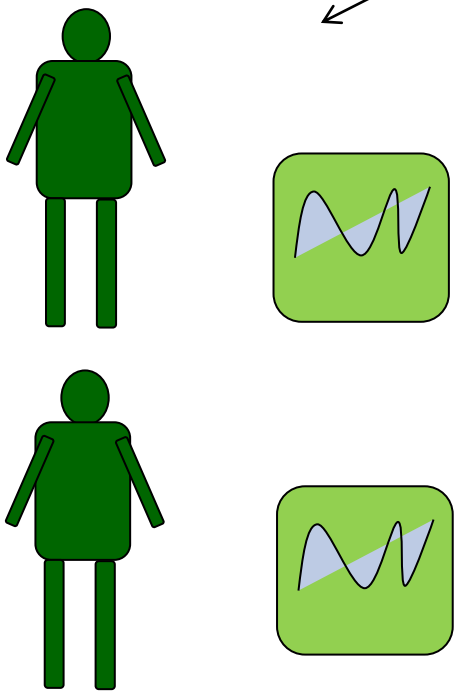
ThermoFisher SCIENTIFIC

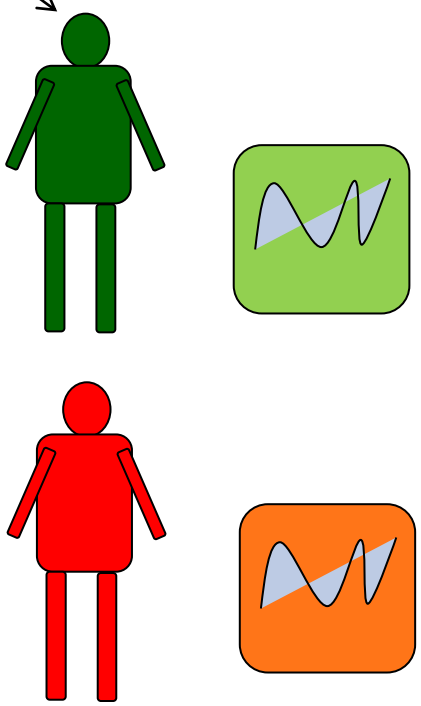
Accuracy/Precision



Anglický termín	Ekvivalent v chemii (do r. 2008)	Ekvivalent VIM3 (od r. 2009)
Measurement trueness	Pravdivost měření	Pravdivost měření
Measurement accuracy	Správnost měření	Přesnost měření
Measurement precision	Přesnost měření	Preciznost měření

Precision

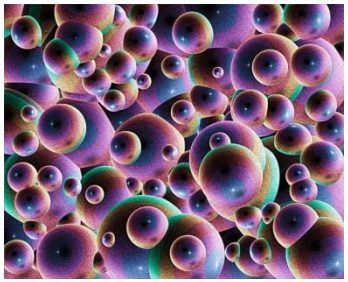




REPEATABILITY:
N x one analyst,
one apparatus

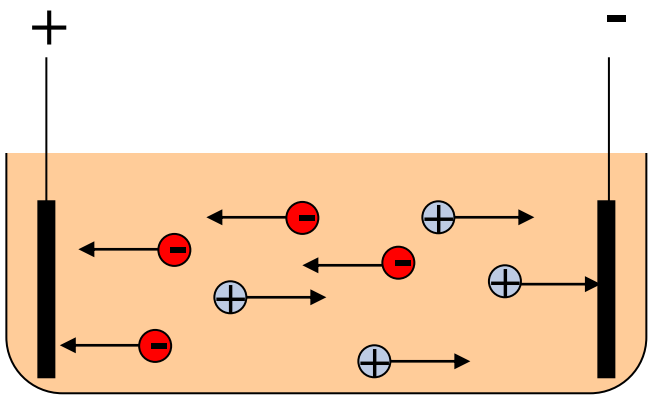
REPRODUCIBILITY:
N x more analysts,
more apparatus

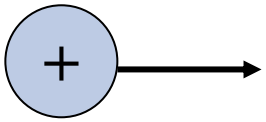
CAPILLARY ELECTROPHORESIS

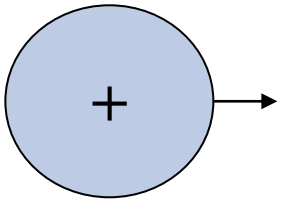


1. **Capillary electrophoresis**– **in general**
2. On the field of separation techniques – **strengths, weakness**
3. Separation of inorganic ions – **examples**
4. Separation of polar and ionic substances – **examples**
5. Chiral separation – **examples**

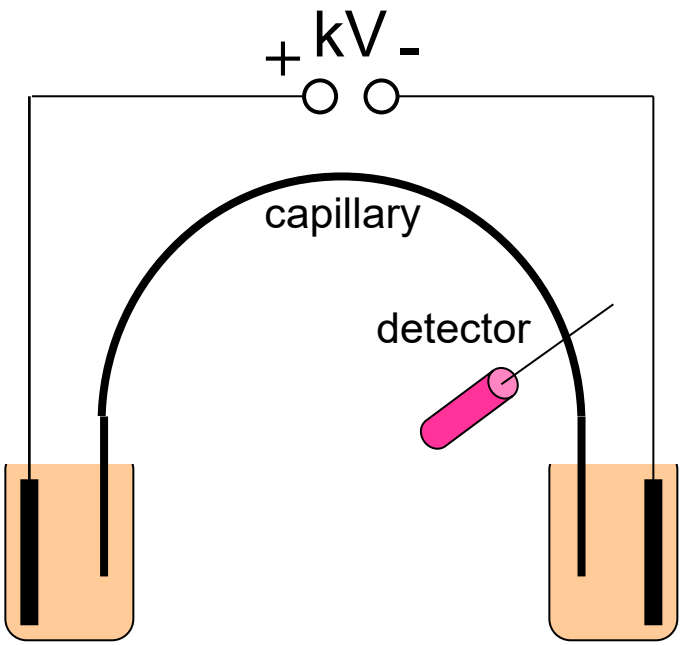
CE



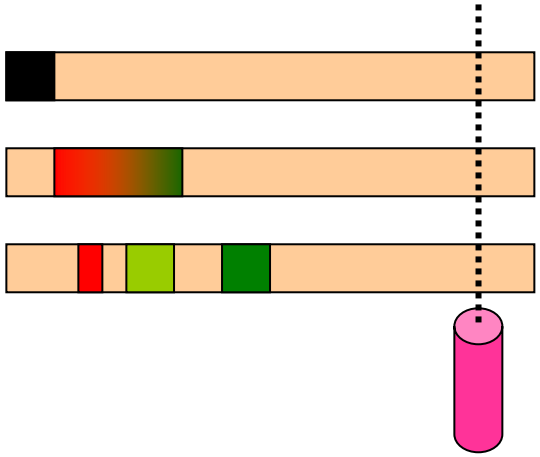


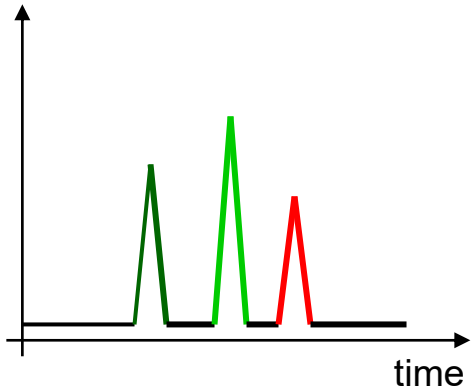


Different velocity (mobility) of ions in el. field



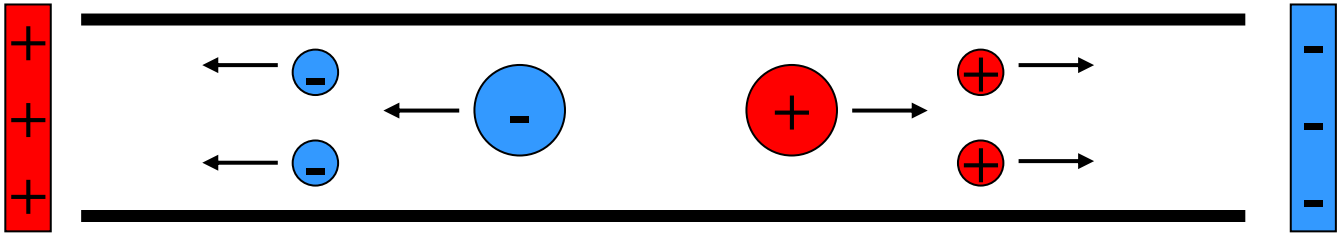
elektrolyt, elektrody





CE, CZE, HPCE

CE - mobility



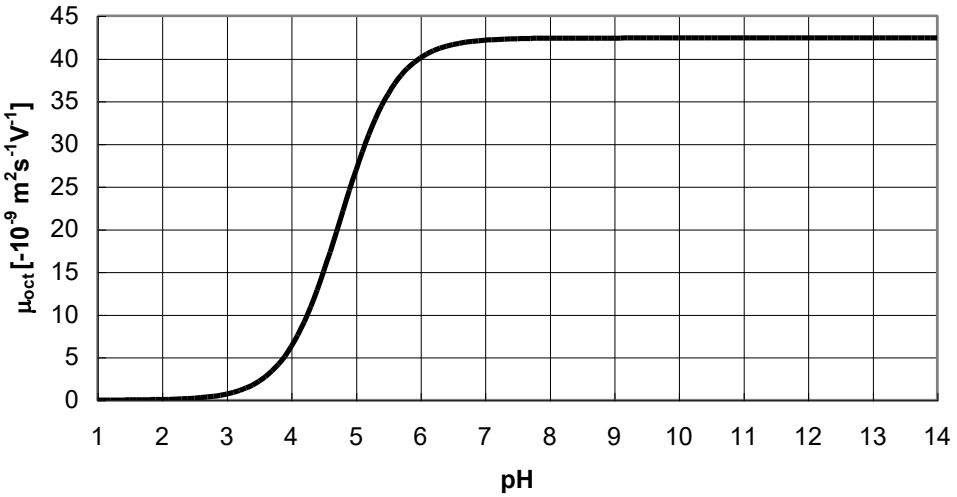
$$v = \mu \cdot E$$

$$\frac{L_d}{t} = \mu \frac{U}{L_c} \Rightarrow t = \frac{L_d L_c}{\mu U}$$

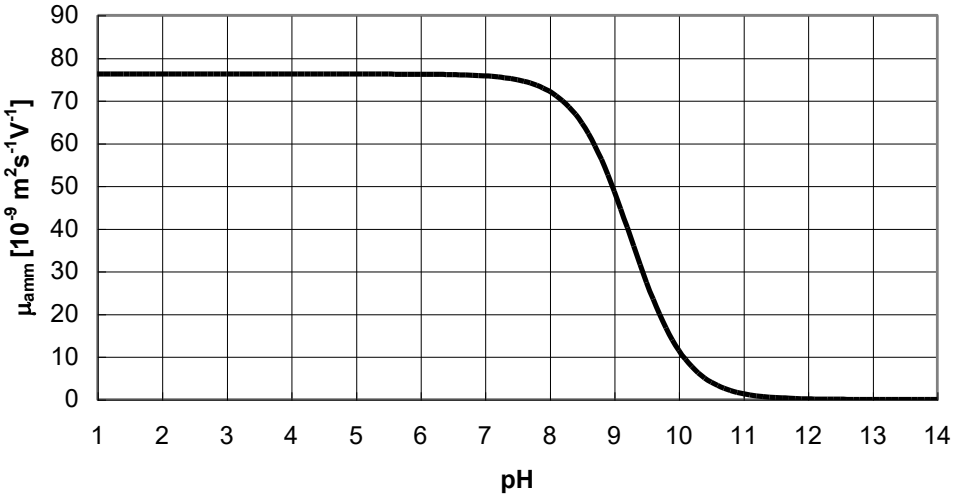
$$\mu = \mu(Q, pK, pH, r, \eta, I, T)$$

CE – dissociation

$$K_a = \frac{[B^-][H^+]}{[HB^+]}$$

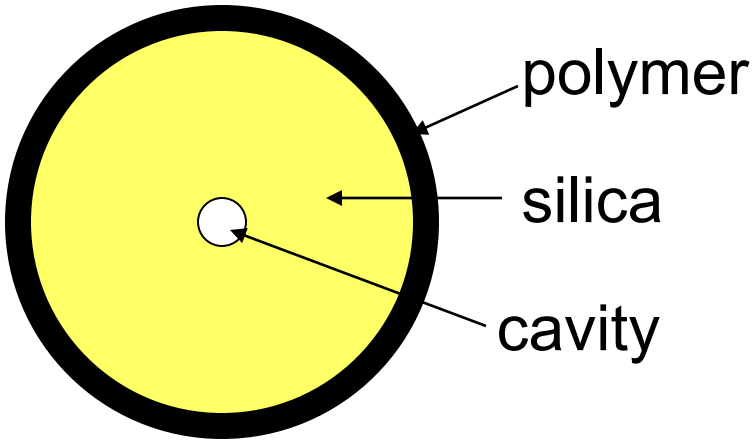


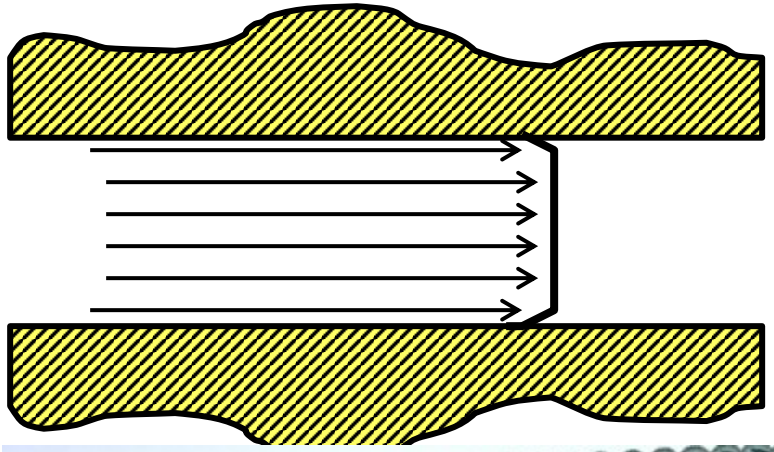
ACETATE ION

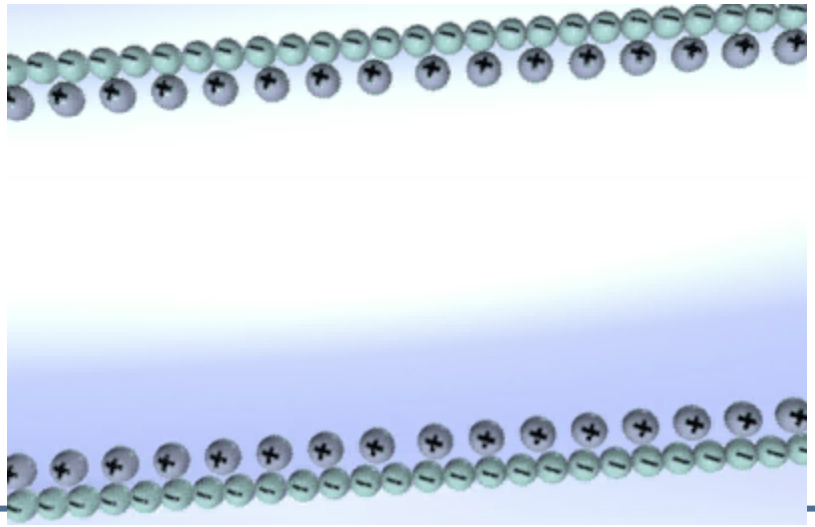


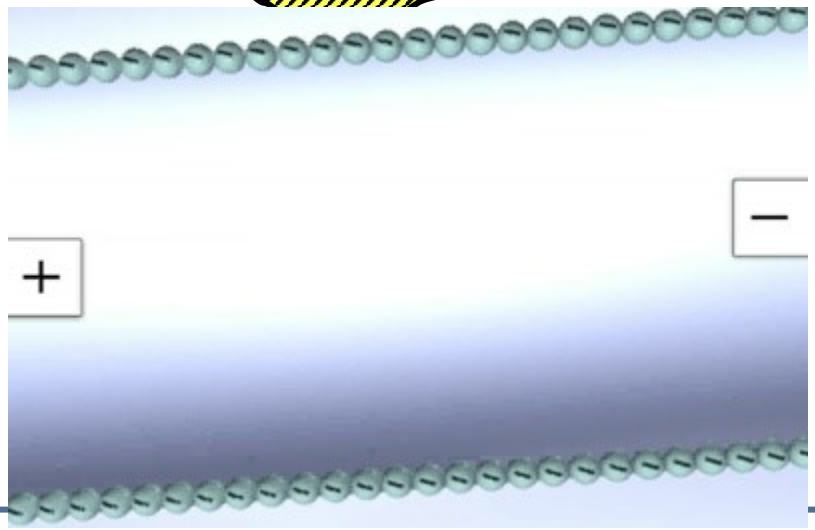
AMMONIUM ION

EOF – (electro)endoosmotic flow ⇒ separation of cations, anions, neutrals during one run





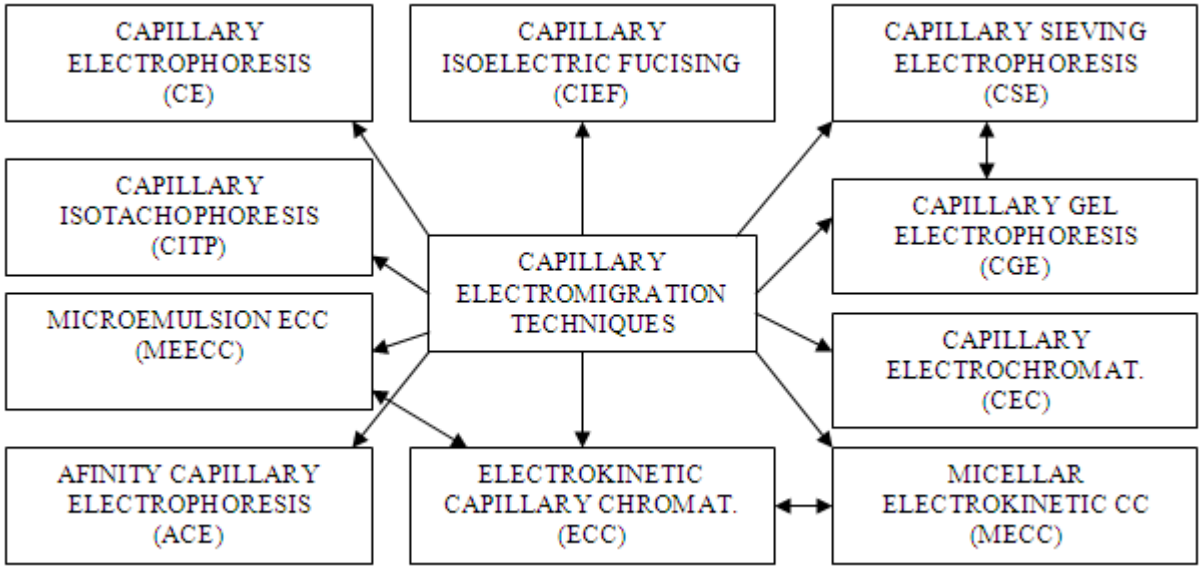




CZE – capillary zone electrophoresis

(M)EKC – (micellar) electrokinetic chromatografy

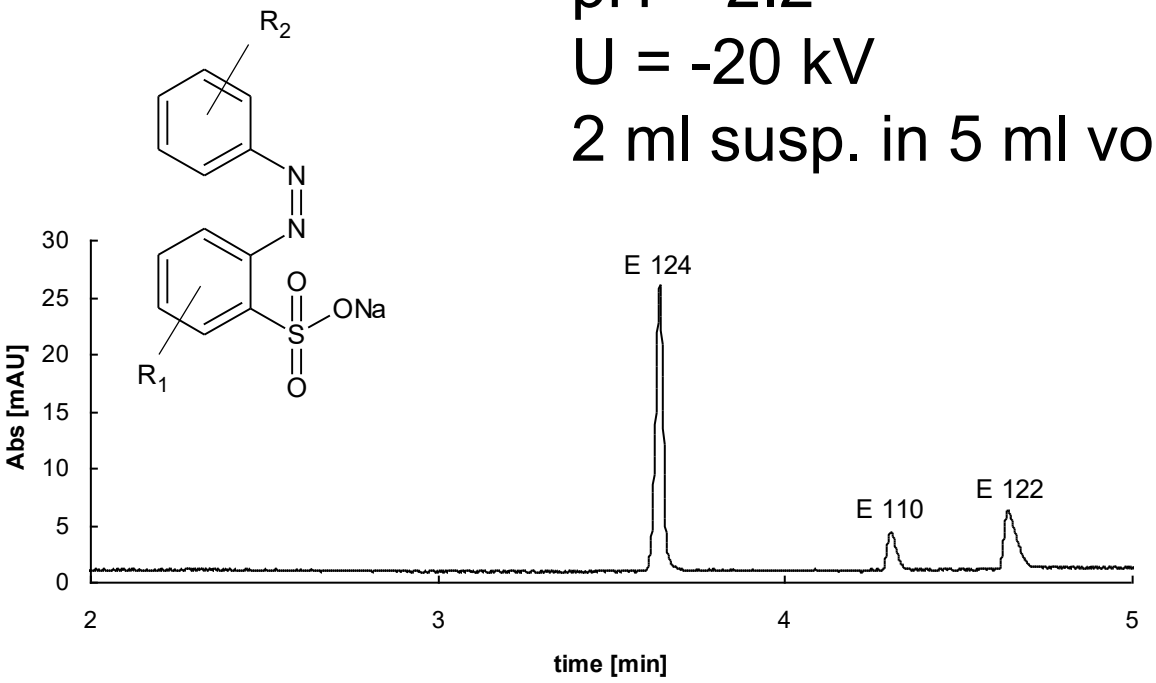
CEC – capillary electrochromatografy



CZE – examples

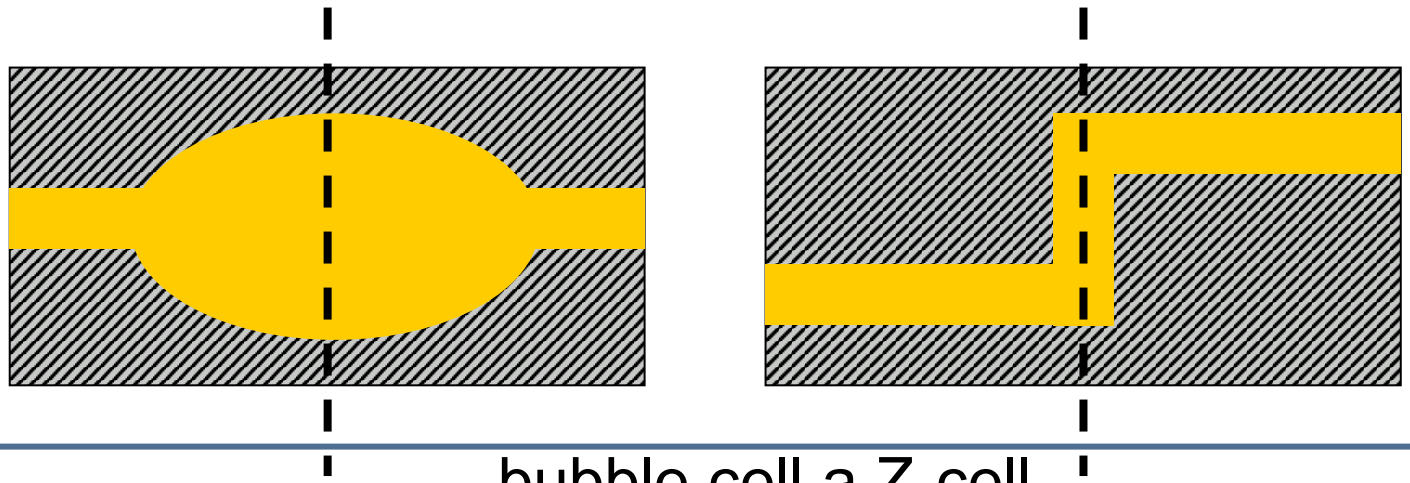
Test of dyes (E124, E110 a E122) in Ibalgin susp.

L_{tot} = 48.5 cm
L_{det} = 40.0 cm
pH = 2.2
U = -20 kV
2 ml susp. in 5 ml vol. flask

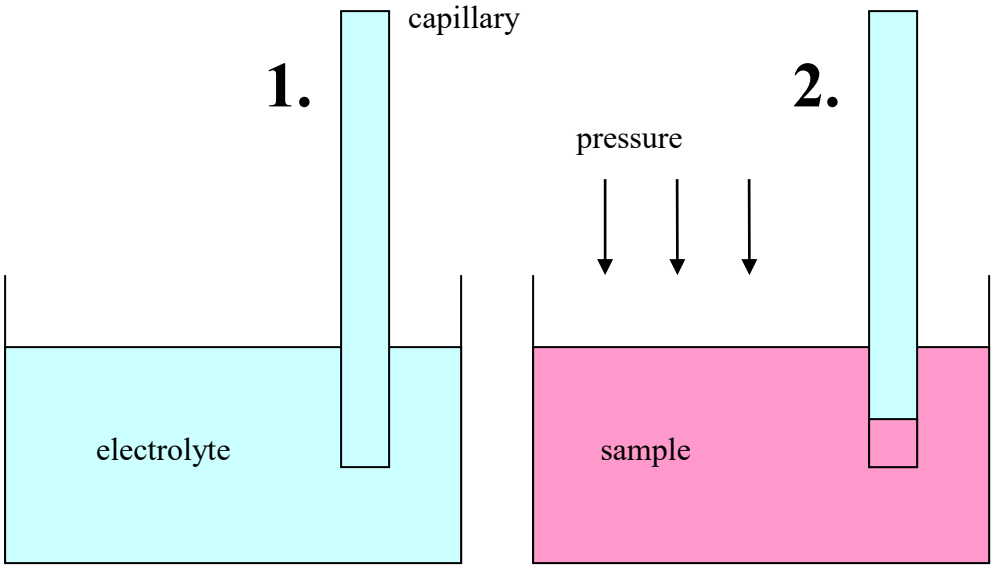


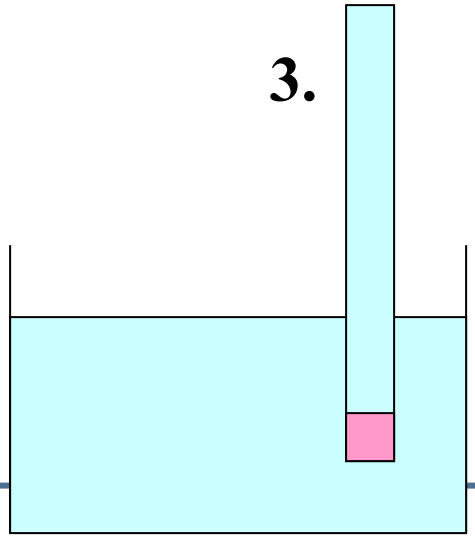
ThermoFisher SCIENTIFIC

- ☑ low running costs compared to GC a HPLC
- ☑ high separation efficiency
- ☑ fast analyses
- ☑ short method development
- ☒ worse robustness and inj. repeatability
- ☒ LOQ ~ 0,1 až 0,2 %
- ☒ Peak area depends on migration time



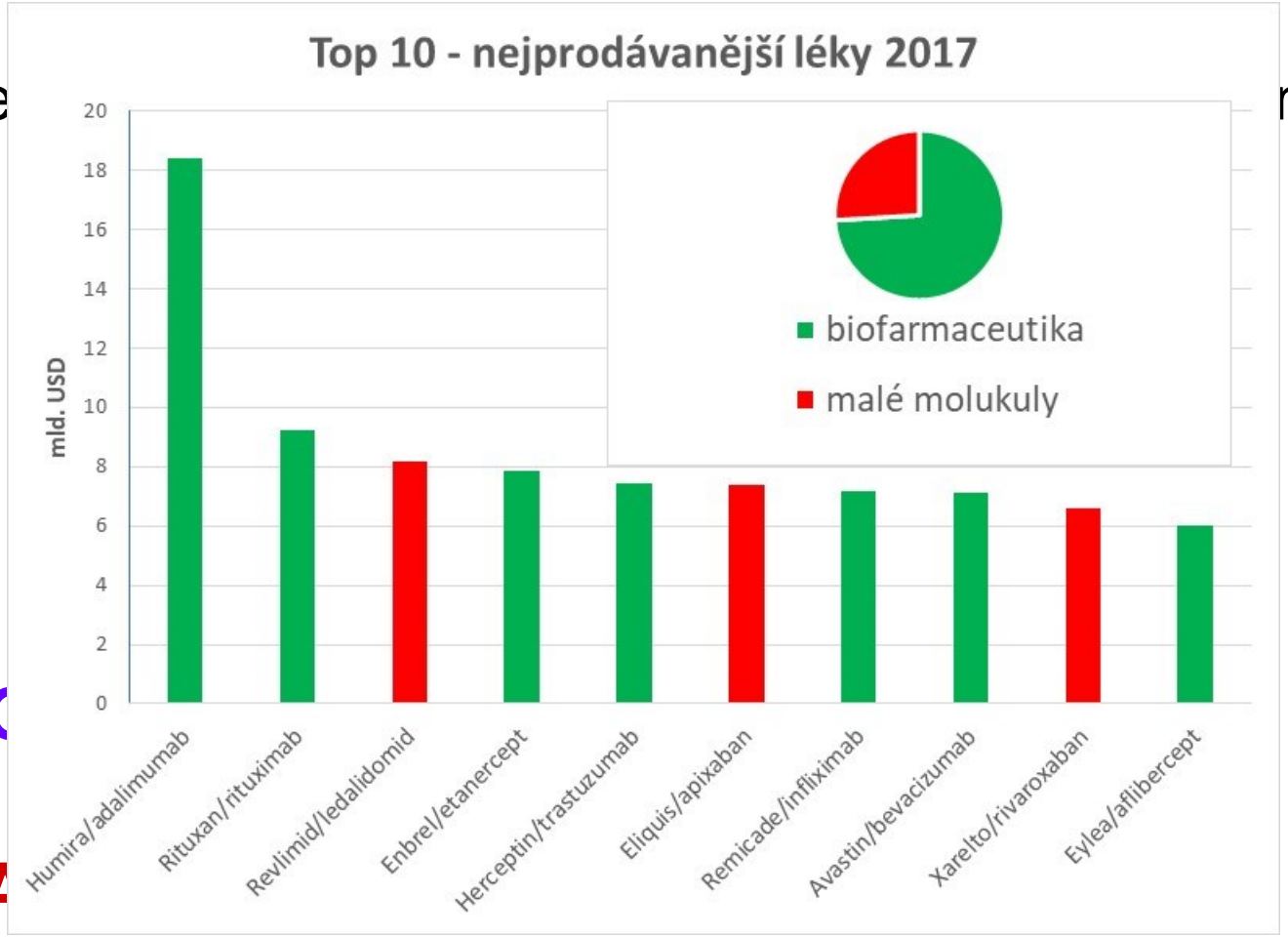
bubble cell a Z-cell





Hydrodynamic injection – the most common in CE

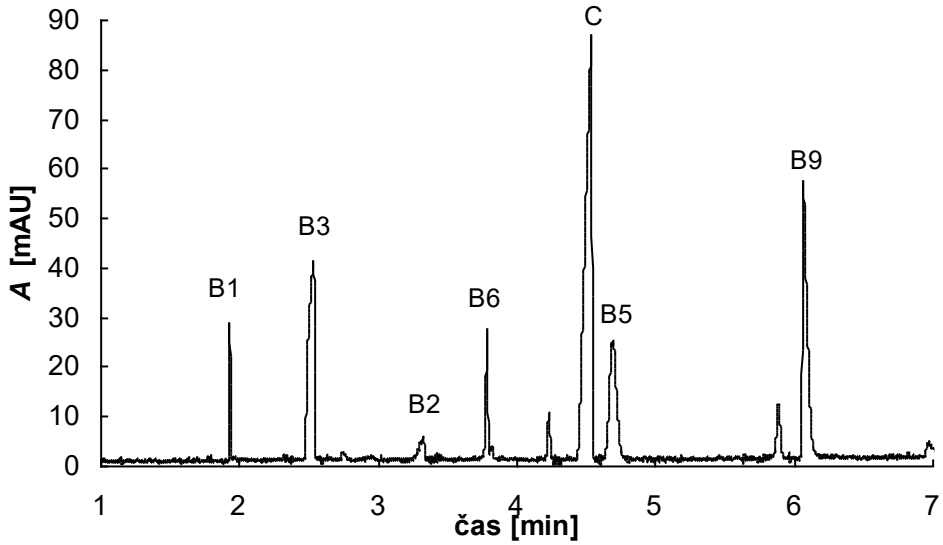
Where we

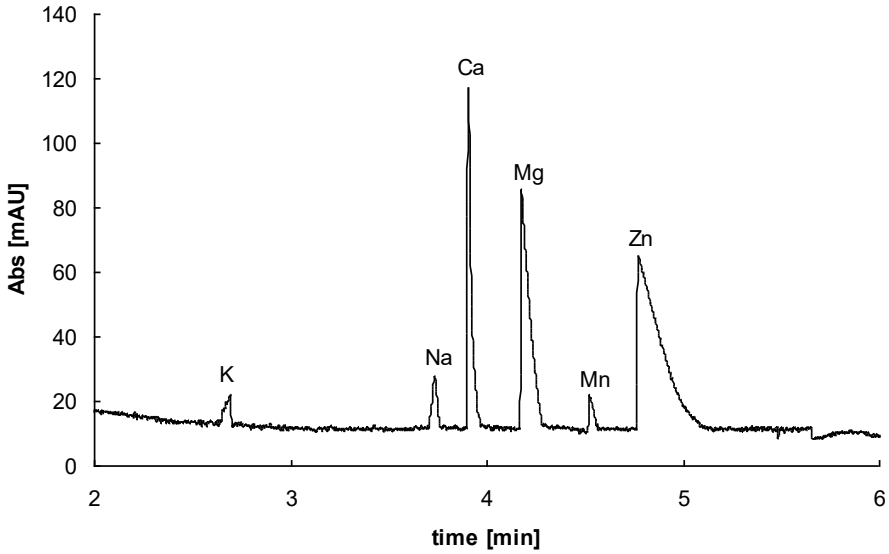


n techs:

- INORG
- IONIC
- CHIRA
- **BIOPHARMA**

CE examples

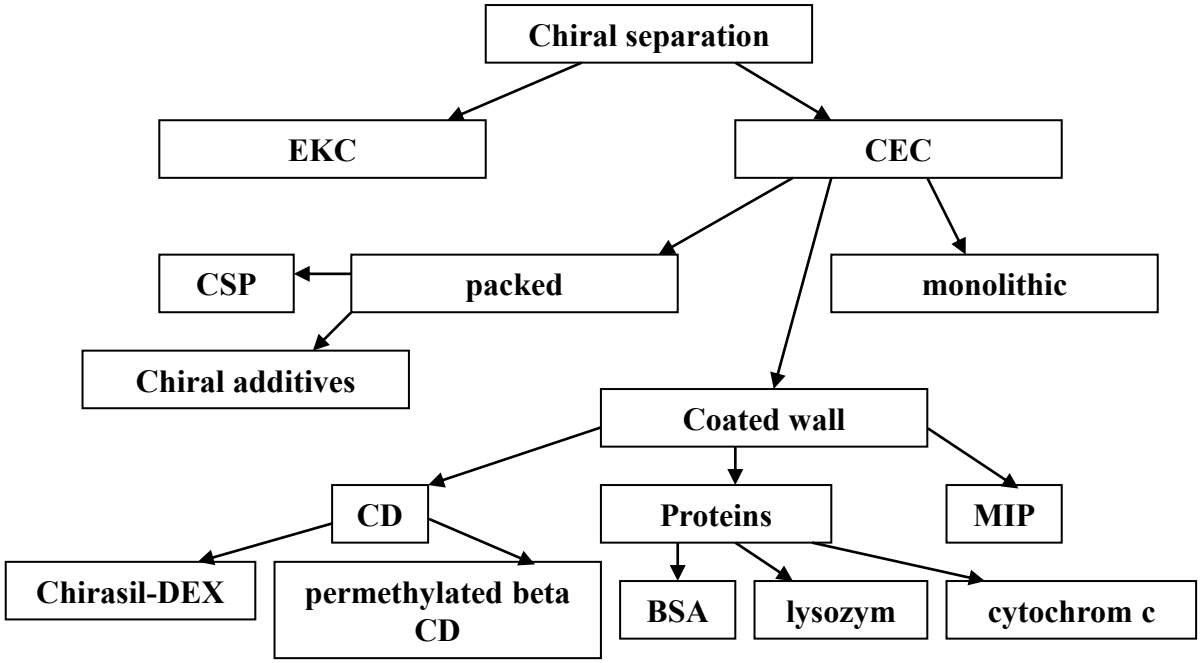


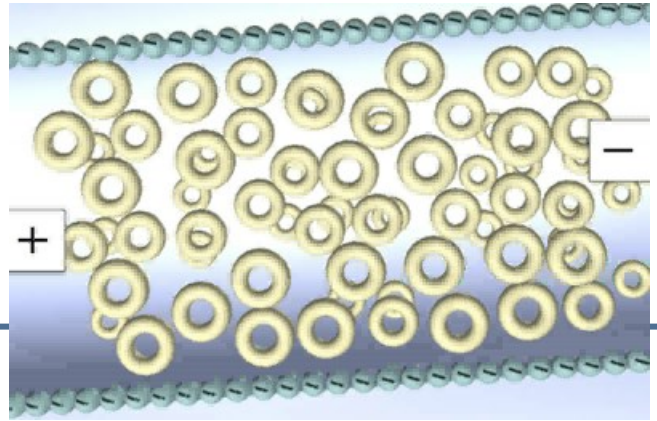


CE examples

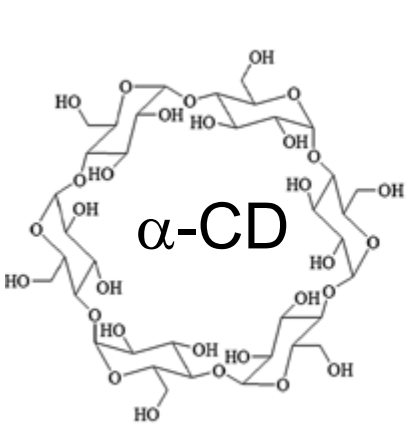
	Omega H3		Geriavit Pharmaton	
component	declared value/cps.	CE*	declared value/cps.	CE*
C	60 mg	✓	60 mg	✓
B1	20 mg	✓	2 mg	✓
B2	5 mg	✓	2 mg	✓
B6	10 mg	✓	1 mg	✓
Nicotinamide	25 mg	✓	15 mg	✓
Calcium pantothenate	10 mg	✓	10 mg	✓
Mg(2+)	30 mg	✓	10 mg	✓
Mn(2+)	2 mg	not found	1 mg	not found
Zn(2+)	15 mg	✓	1 mg	not found

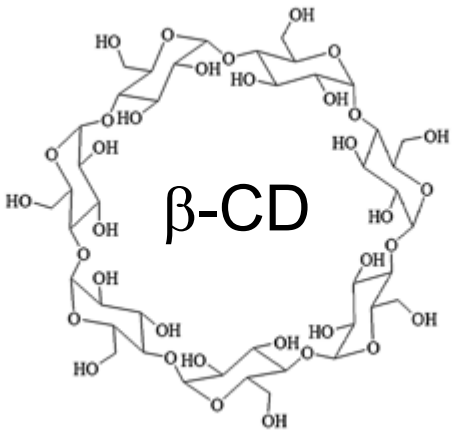
CE chiral separation

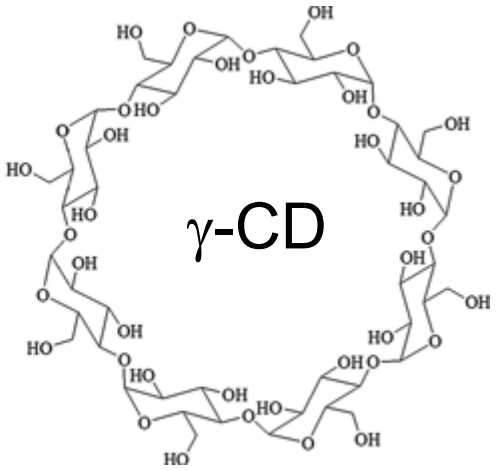




CE chiral separation

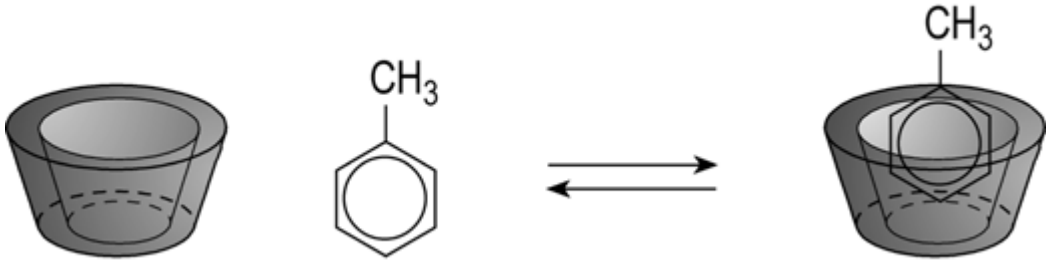






!

6, 7 a 8 glucopyranose units

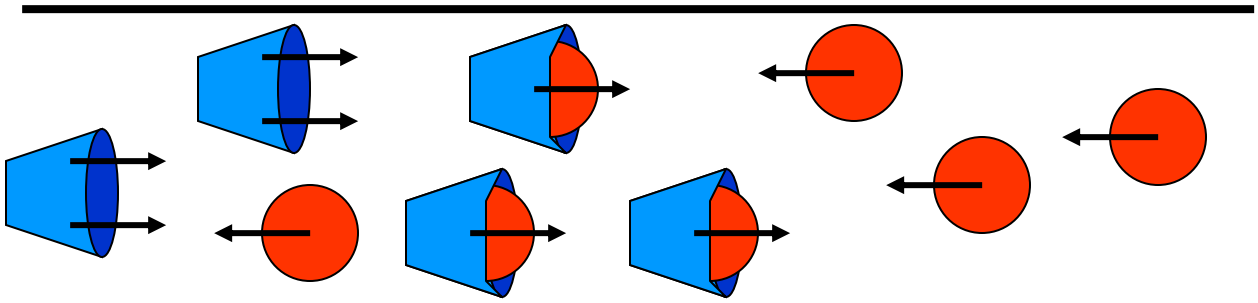


selector analyte complex

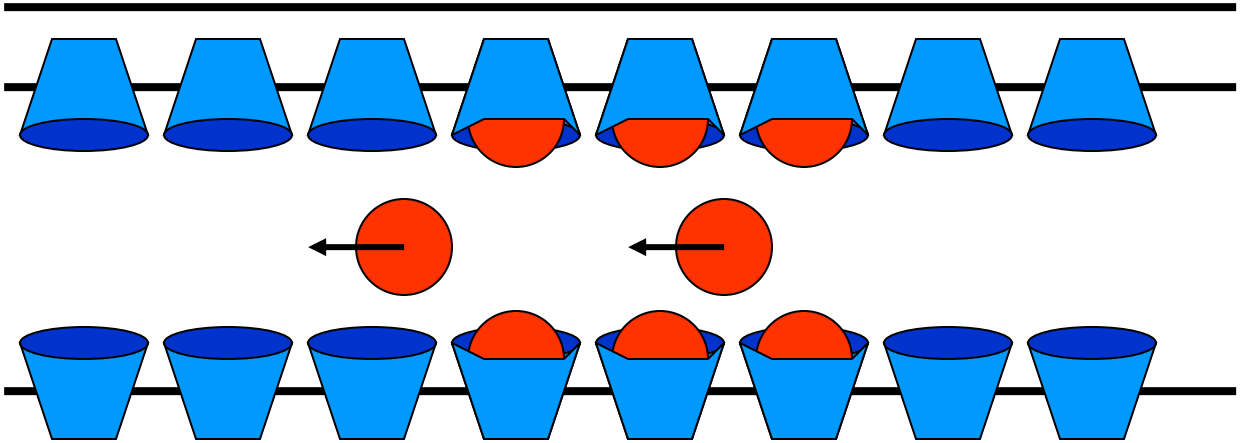
- hydrophilic surface and hydrophobic inert part of cavity
- derivatisation => positive/negative charged selector

CE chiral separation

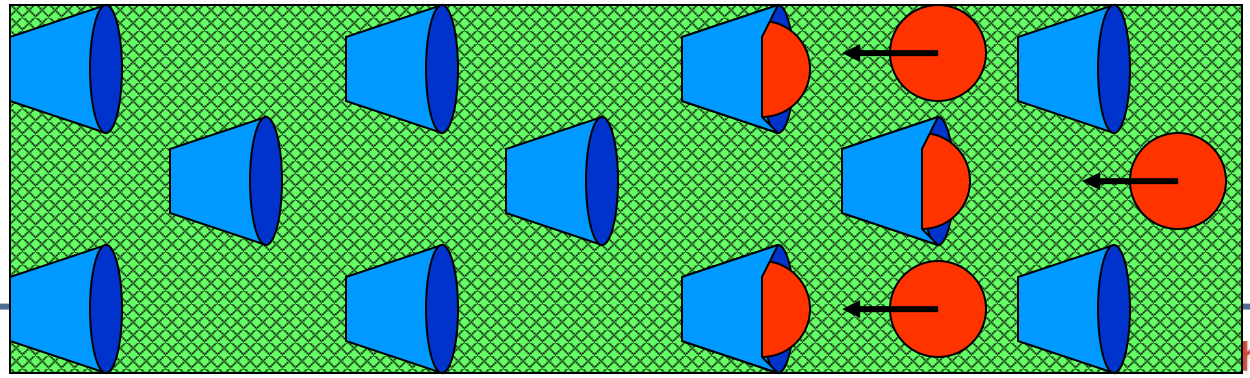
Addition into BGE



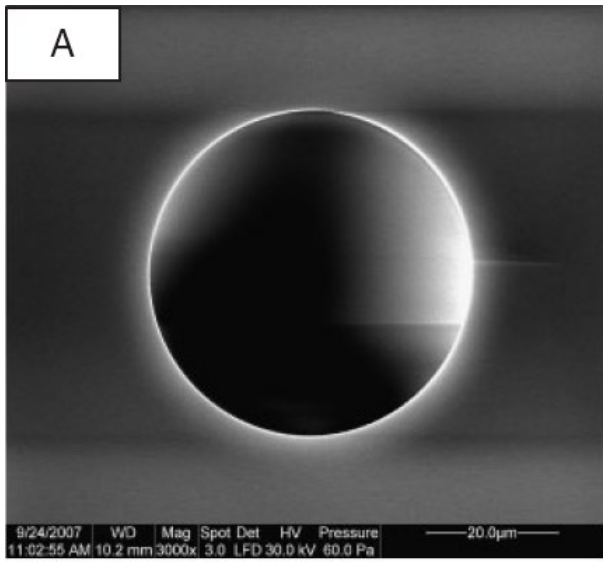
OT-CEC

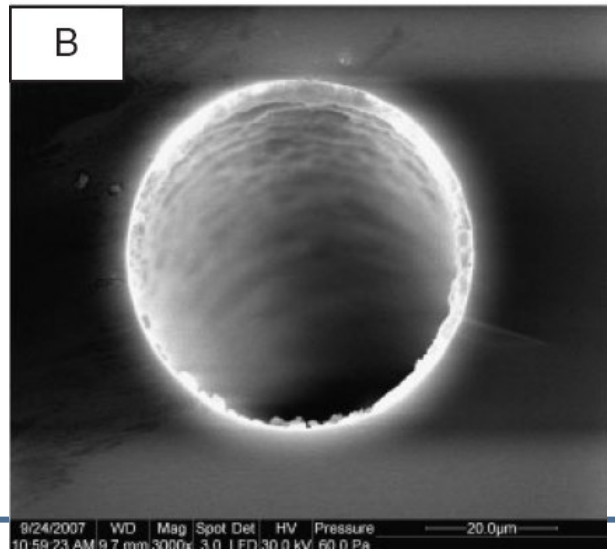


packed and monolithic CEC



CE chiral separation



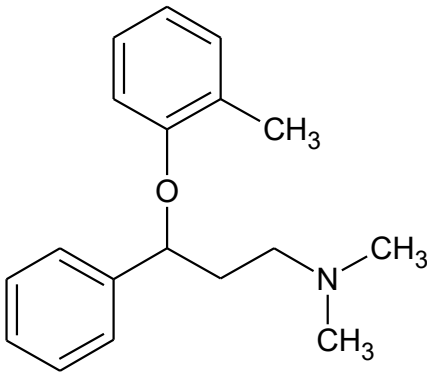


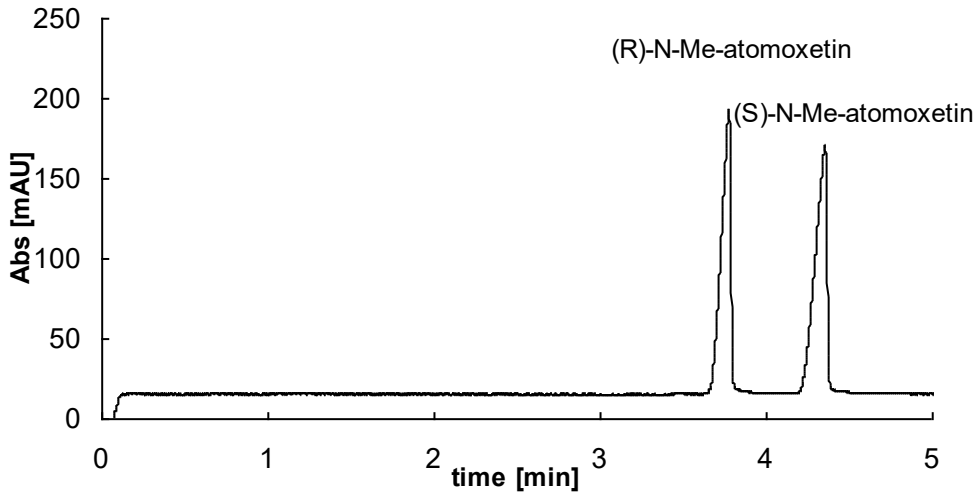
A: silica capillary
B: „coated“ silica capillary (OT-CEC)

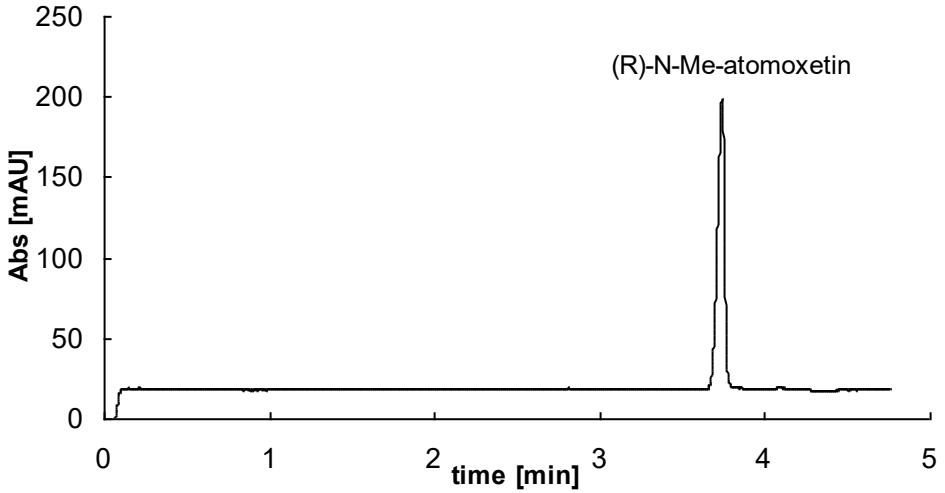
Electrophoresis 2008, *29*, 3933–3940

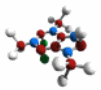
ThermoFisher SCIENTIFIC

CE chiral separation

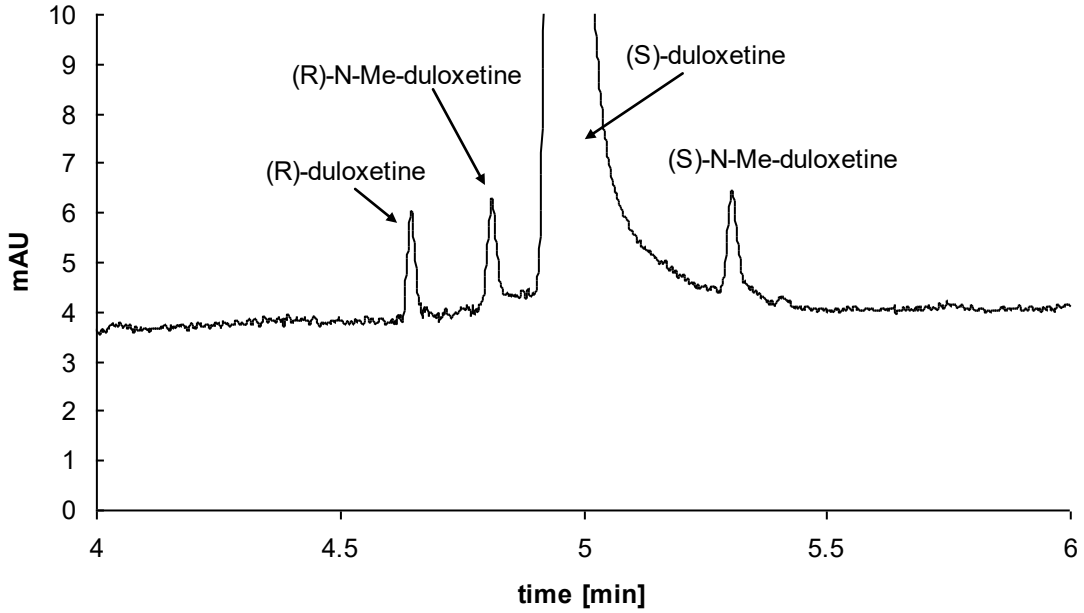


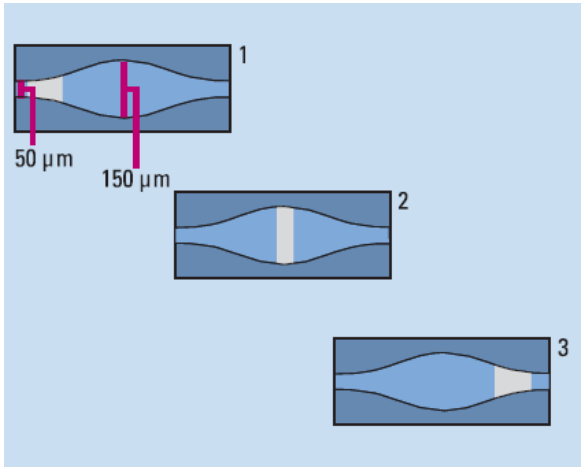


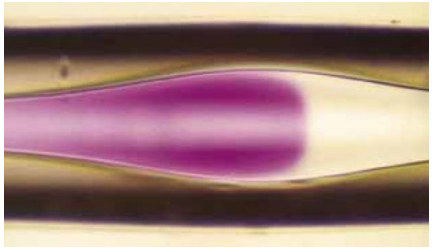




CE chiral separation





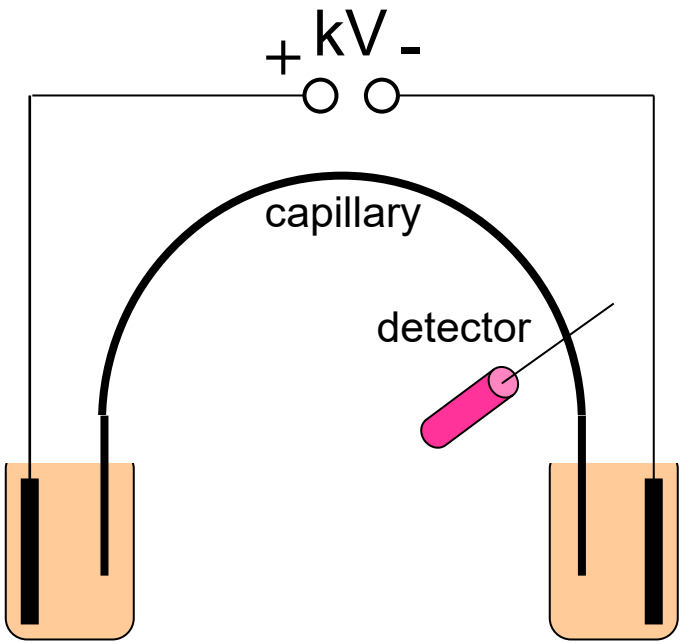


Limit of detection (LOD) and limit of quantitation (LOQ)
The limit of detection has been calculated by the formula:

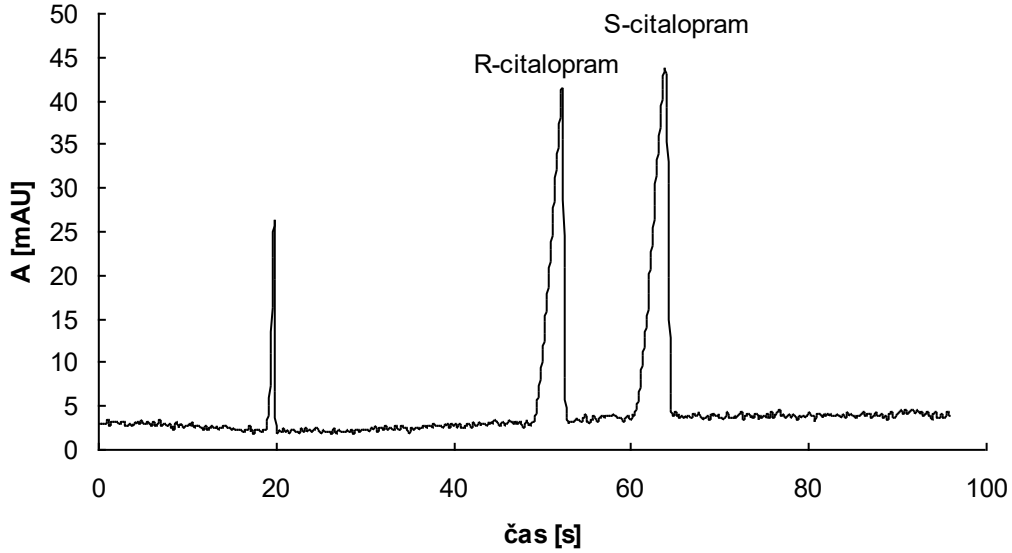
$$\mathrm{LOD} = \frac{3.3 \cdot \sigma}{S}$$

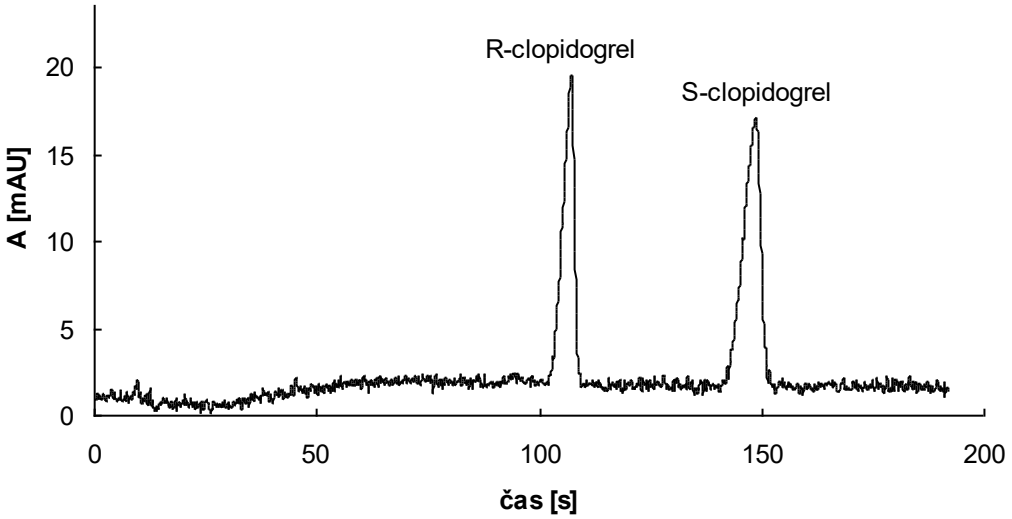
σ is ASTM noise of baseline value (0.138 mAU)
S is the slope of regression line - (11.0 mAU/%)
The detection limit of (R)-duloxetine has been 0.04 % on current condition
The quantitation limit is triple of this value, i.e. 0.12 %

CE chiral separation

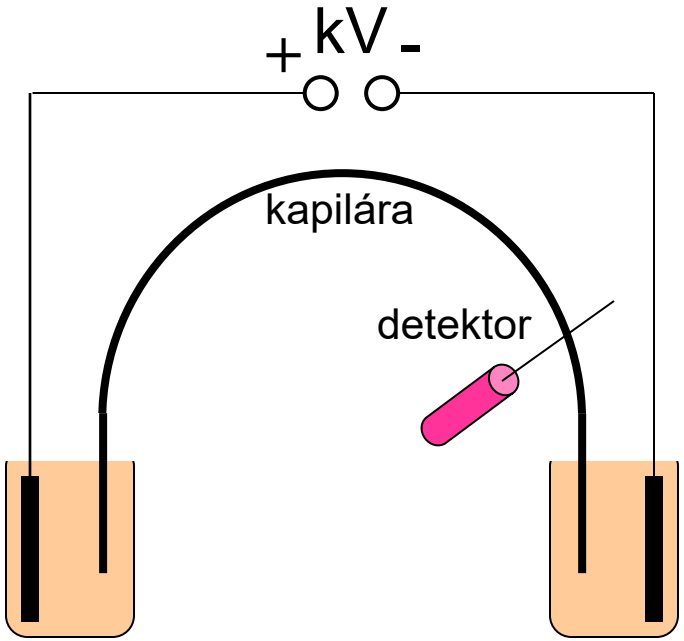


electrolyte, electrodes

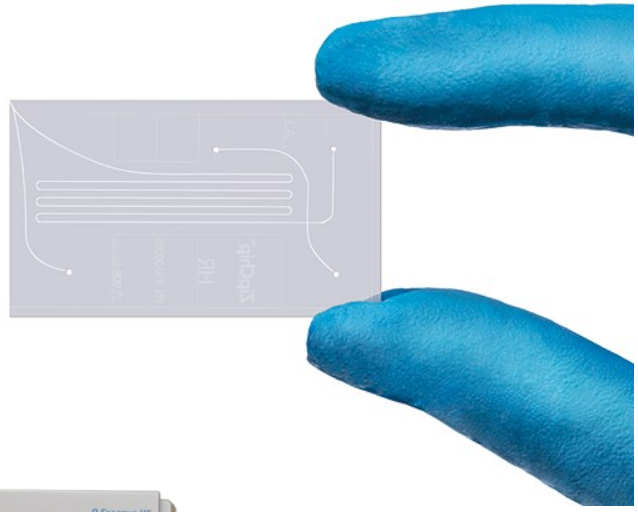




CE biopharma



elektrolyt, elektrody



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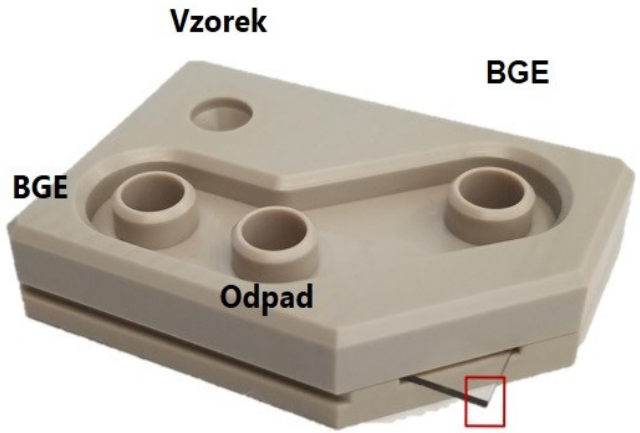
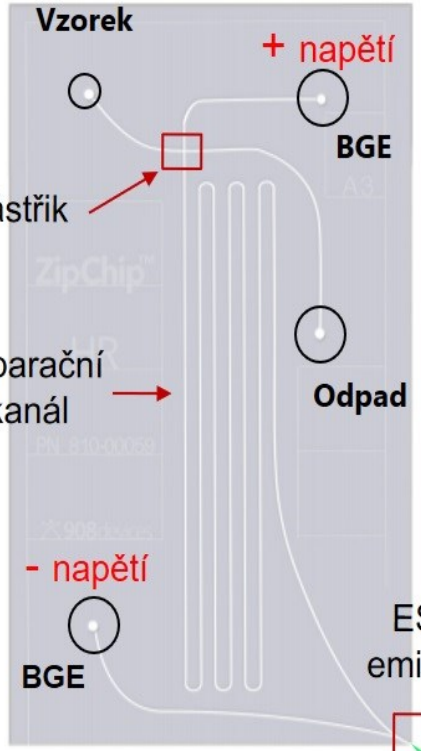
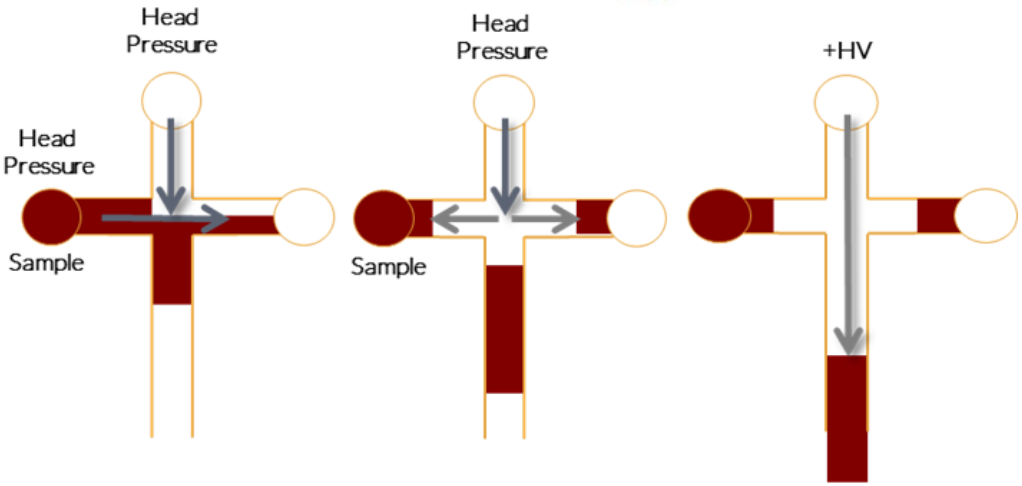
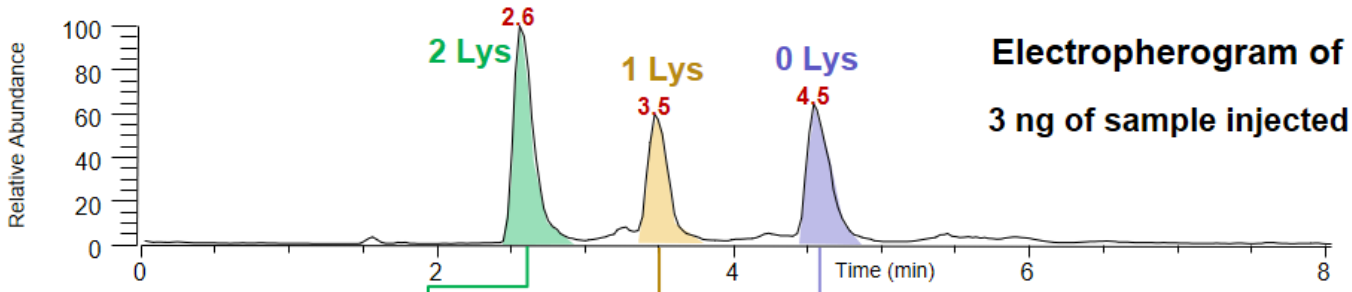
CE biopharma







CE biopharma

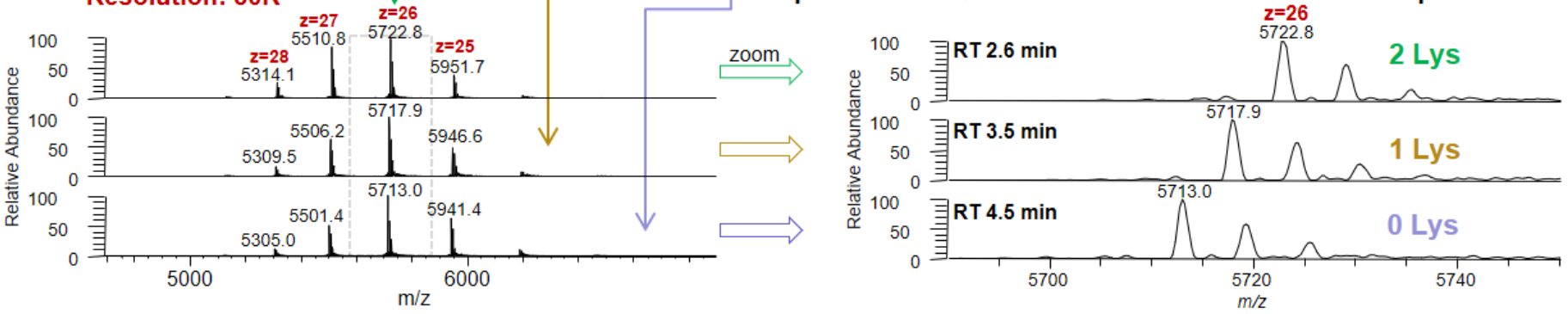


Electropherogram of intact infliximab:

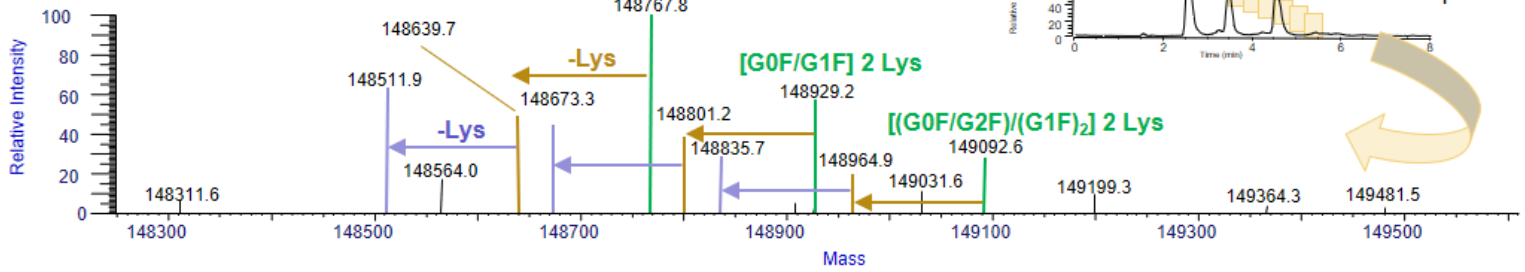
3 ng of sample injected

Resolution: 30K

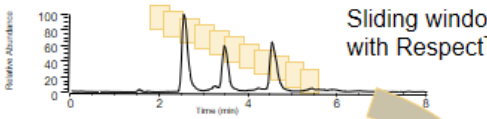
Full MS spectra from Q Exactive HF-X MS with BioPharma Option



Deconvoluted MS spectrum

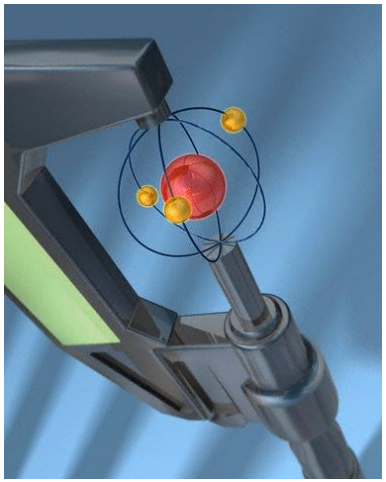


Sliding window deconvolution with Respect™ algorithm

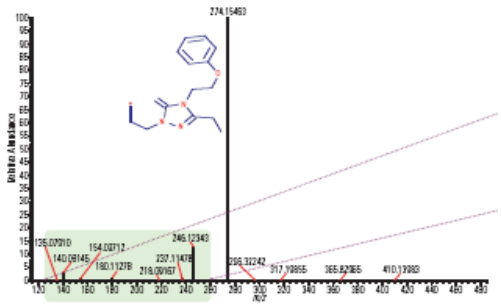


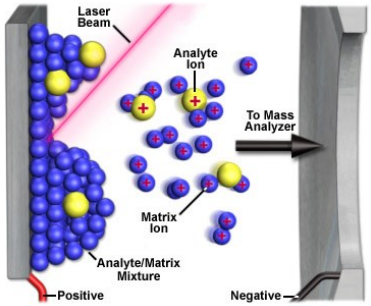
ThermoFisher SCIENTIFIC

MASS SPECTROMETRY



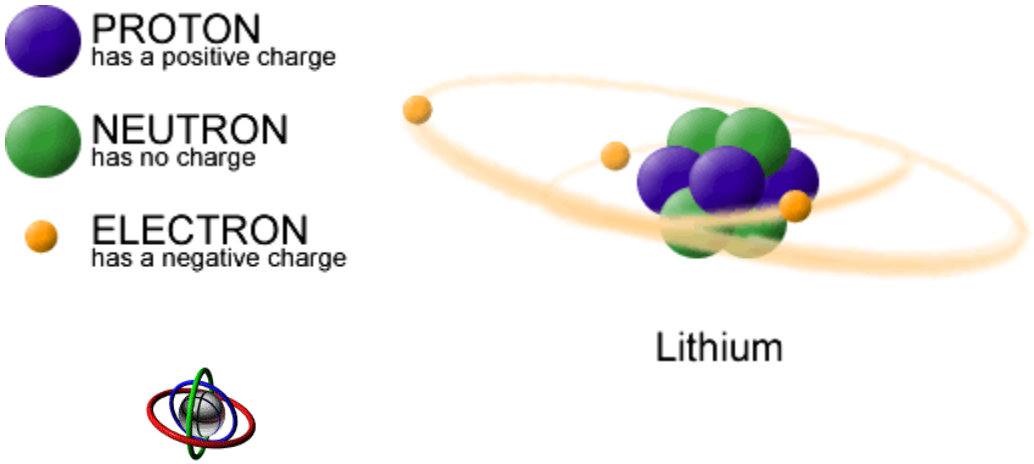
1. **Mass spectrometry** – **in general**
2. Qual/Quan approach on MS
3. Hyphenated MS (GC-MS, LC-MS)
4. Configuration of MS
5. Structural analysis in Pharmacy - **examples**



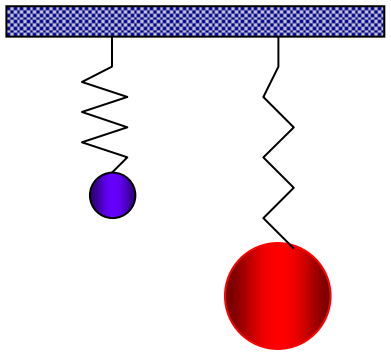


MS – mass spectrometry

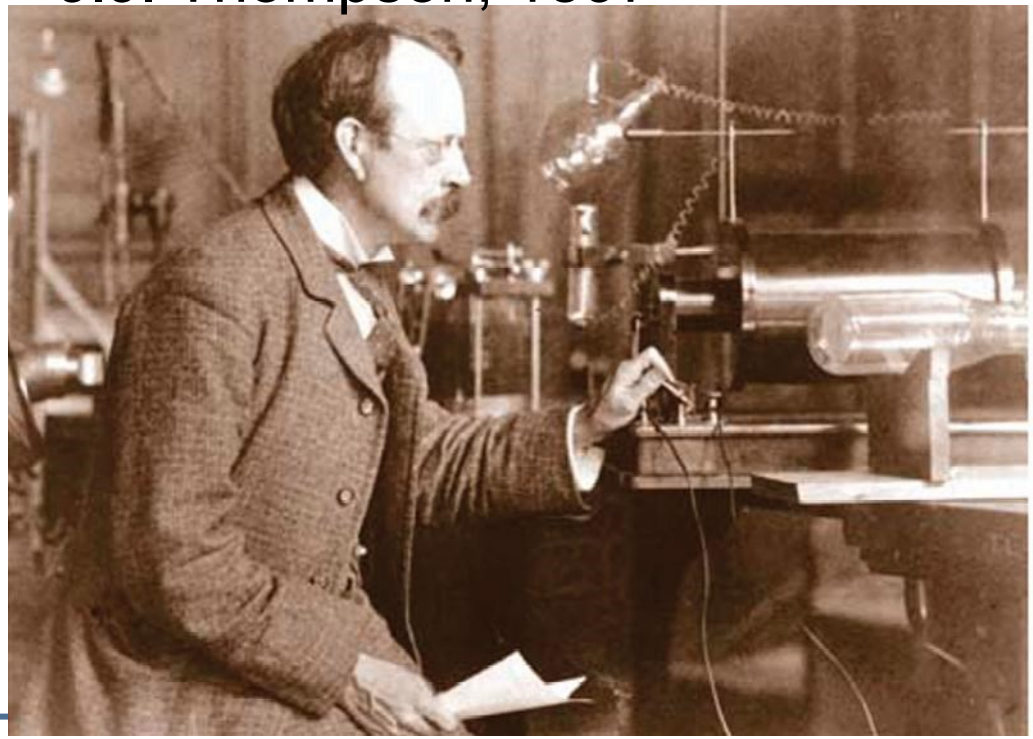
Analytical techniques that measures mass-to-charge ratio

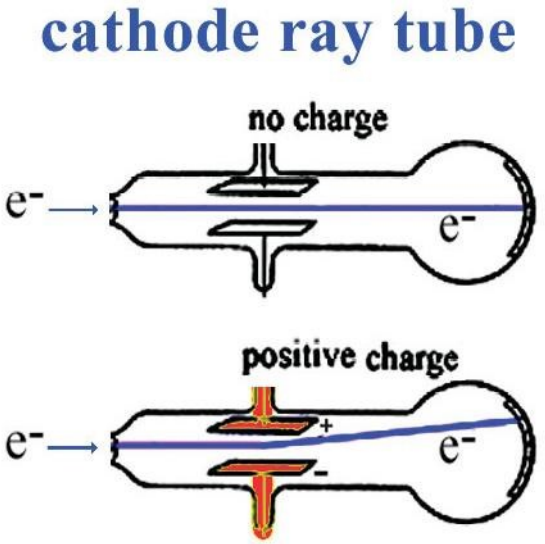


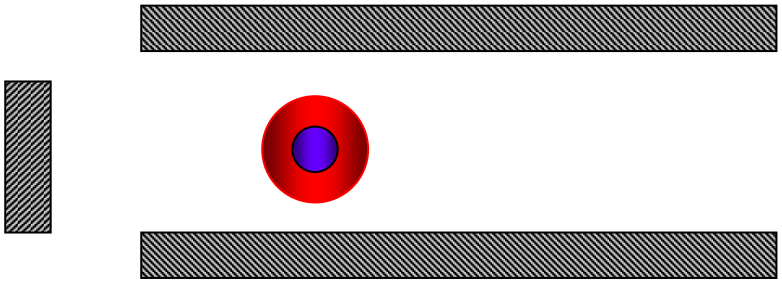
$$m \cdot g = k \cdot \Delta l$$

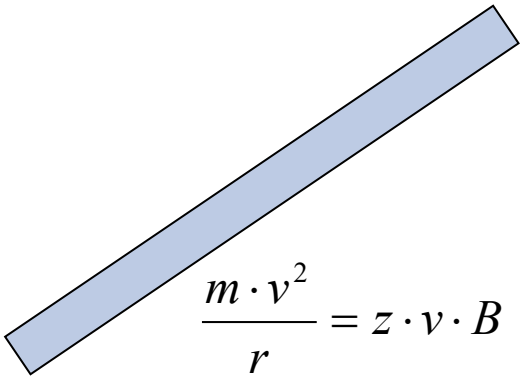


J.J. Thompson, 1897

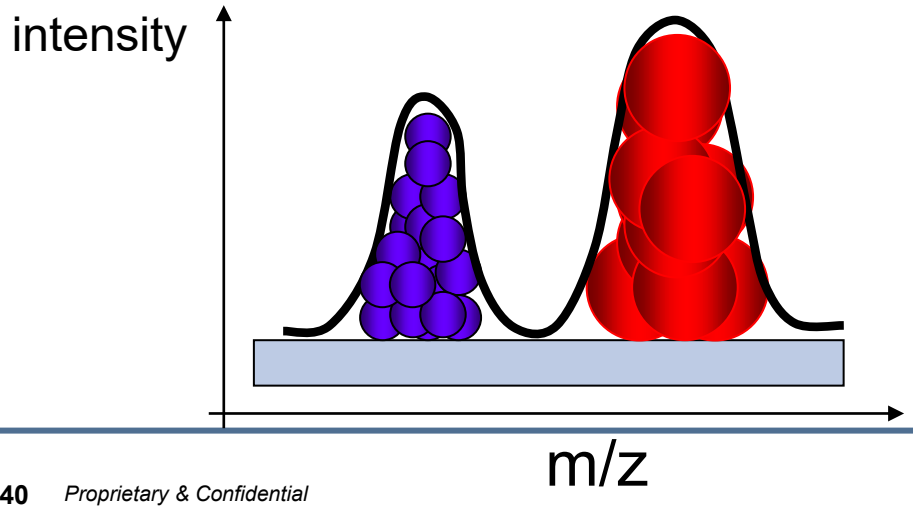


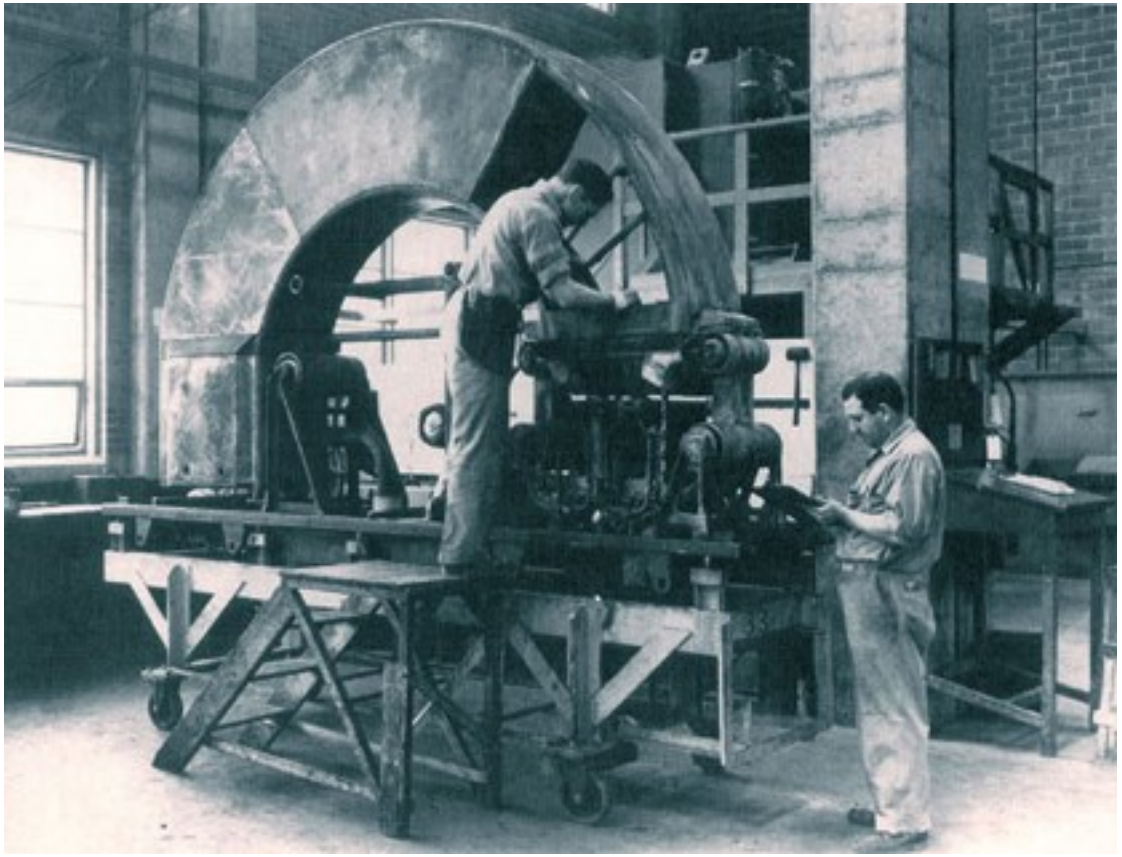






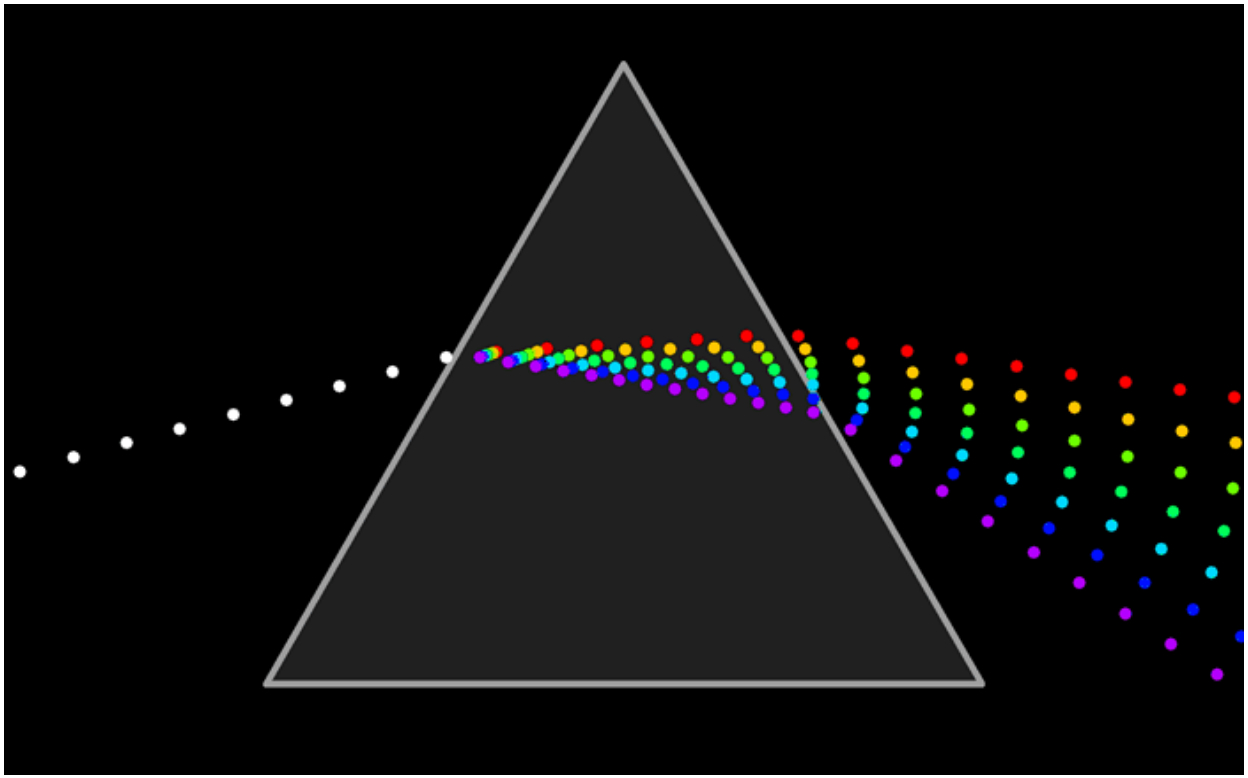
$$\frac{m \cdot v^2}{r} = z \cdot v \cdot B$$



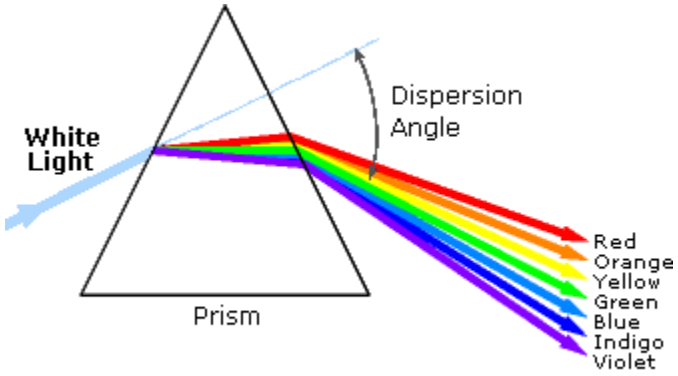


1942: Calutron – separation of ^{235}U a ^{238}U

Light dispersion – visible range – by the prism



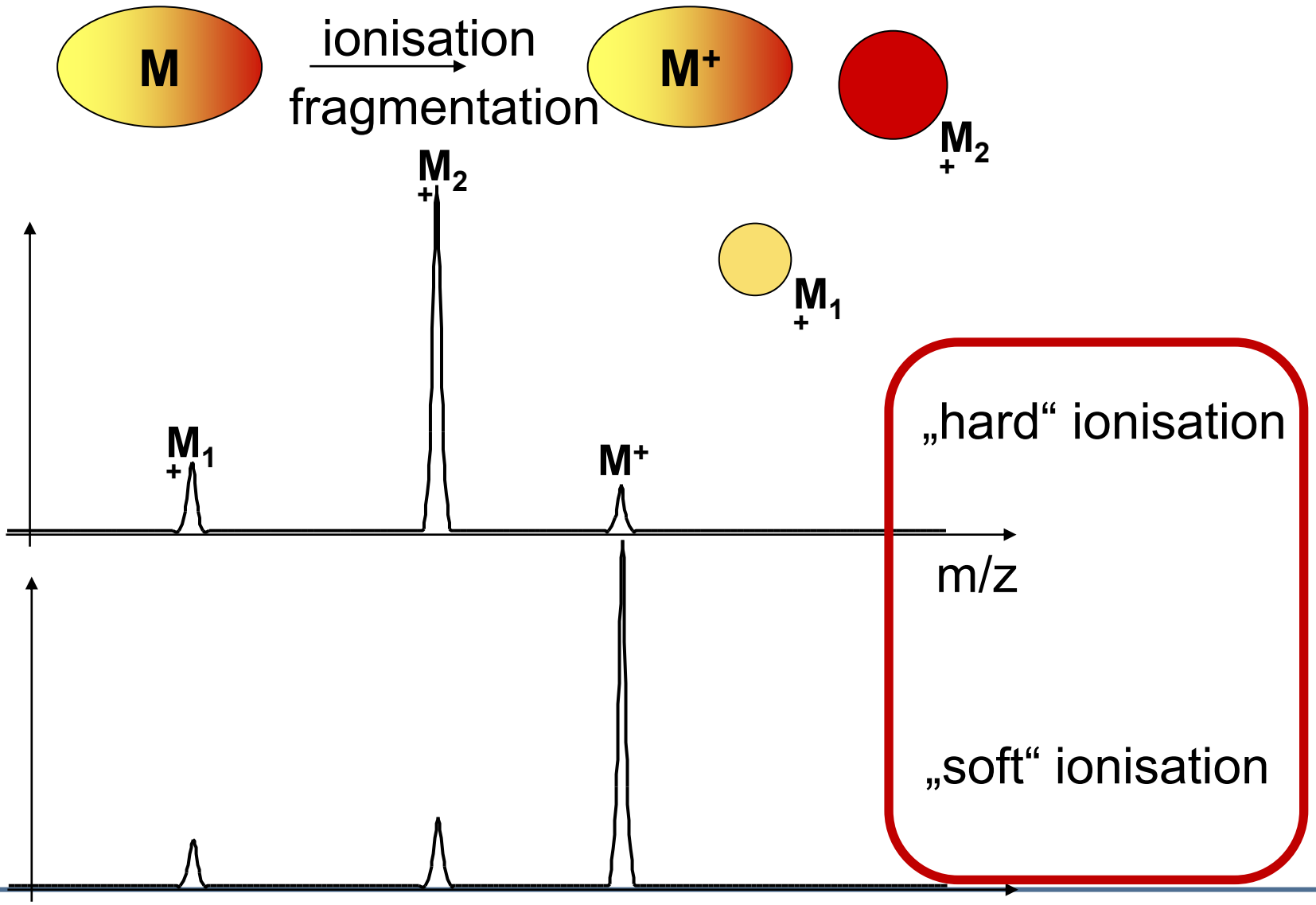
„borrowing“ term SPECTRUM…SPECTROMETRY



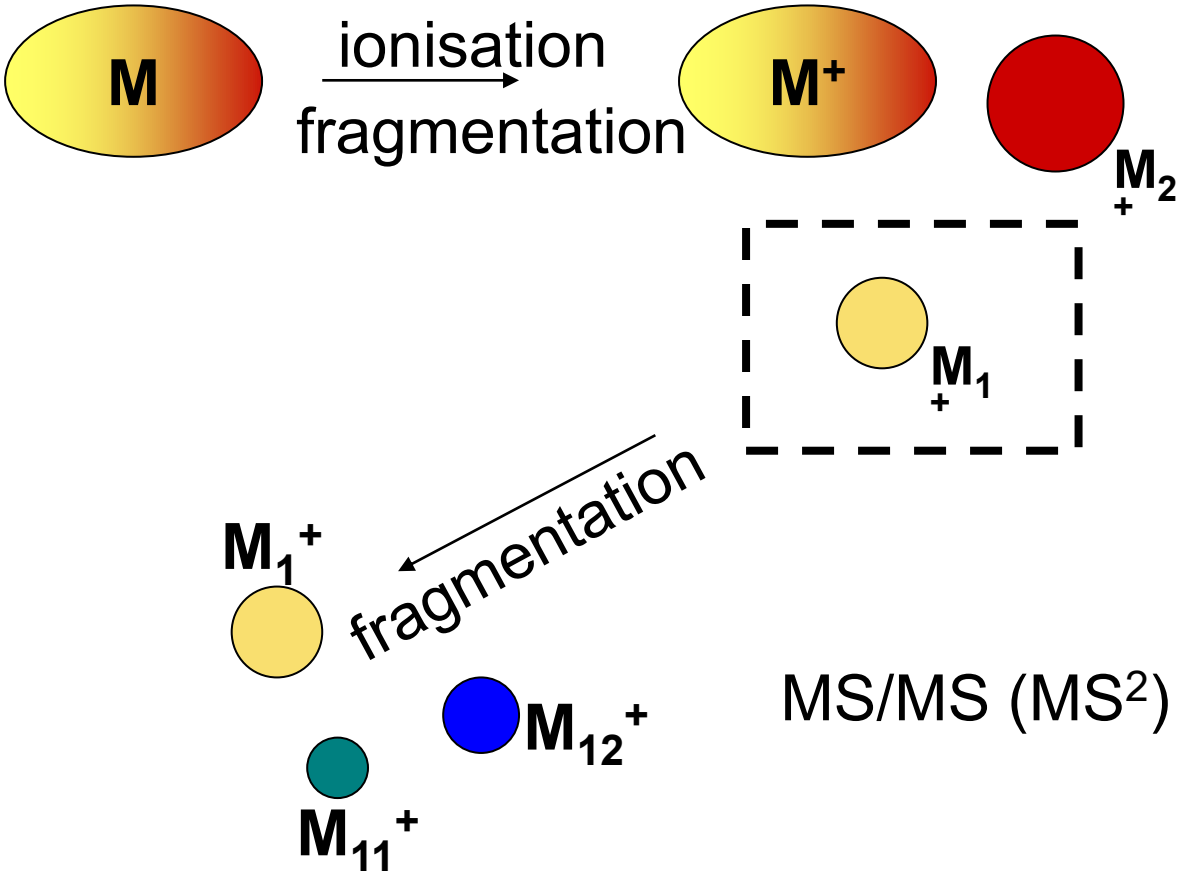
Dispersion with prism
- formation of elmg. spectrum

Separation of ions in mag. field
- formation of mass spectrum

Ionisation

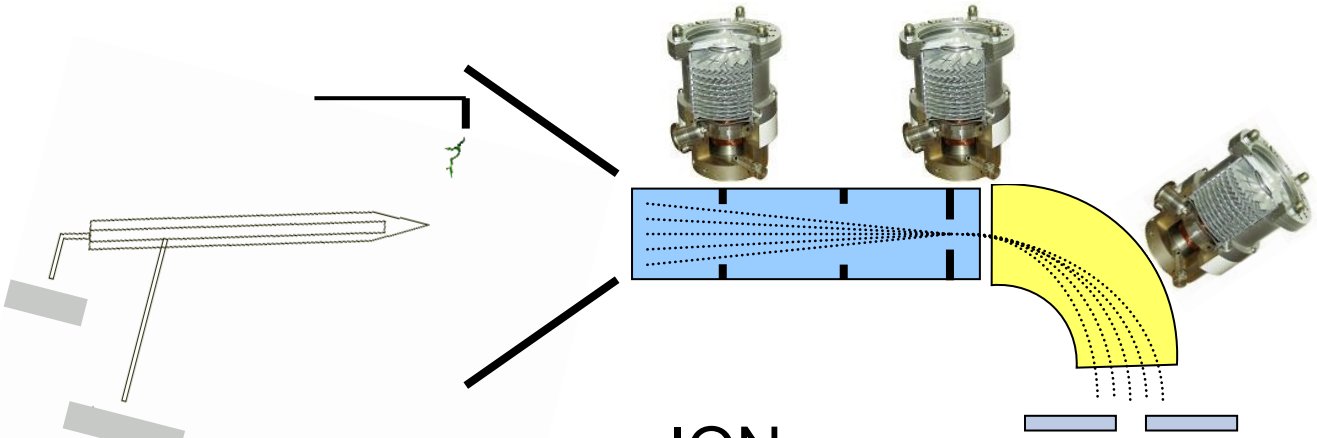


MS^n



Instrumentation

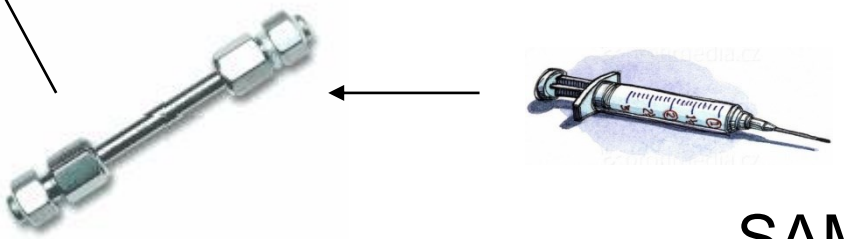
TURBOMOLECULAR PUMPS



ION SOURCE

ION OPTICS

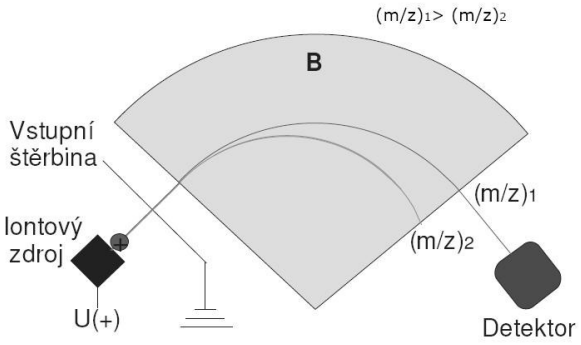
ANALYZER + MULTIPLIER

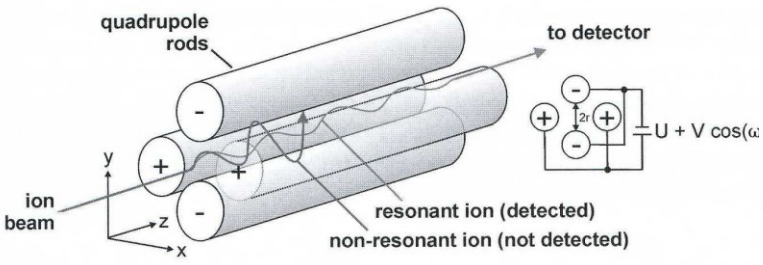


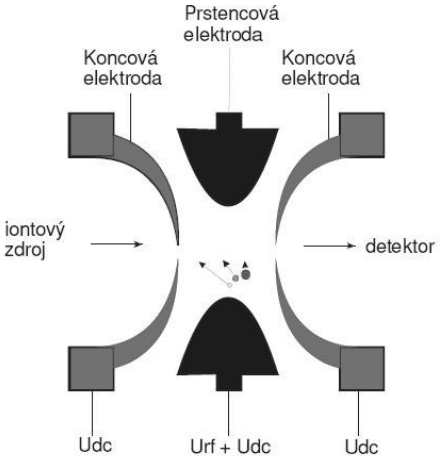
SEPARATION (HPLC, GC, CE)

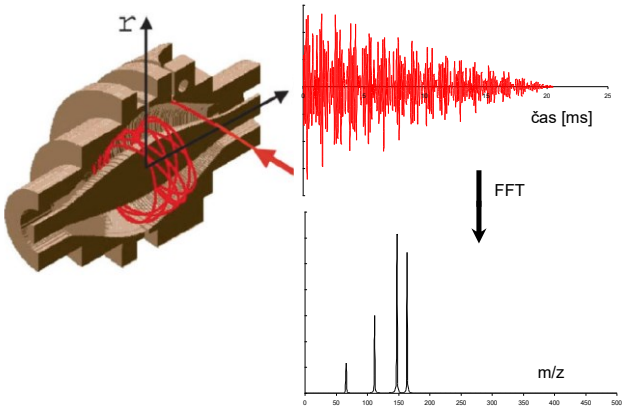
SAMPLE (MIXTURE)

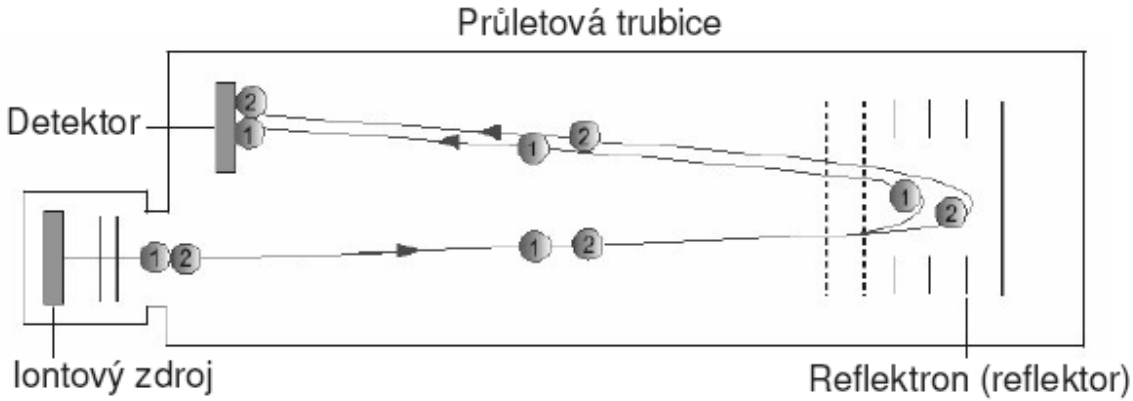
Analyzers





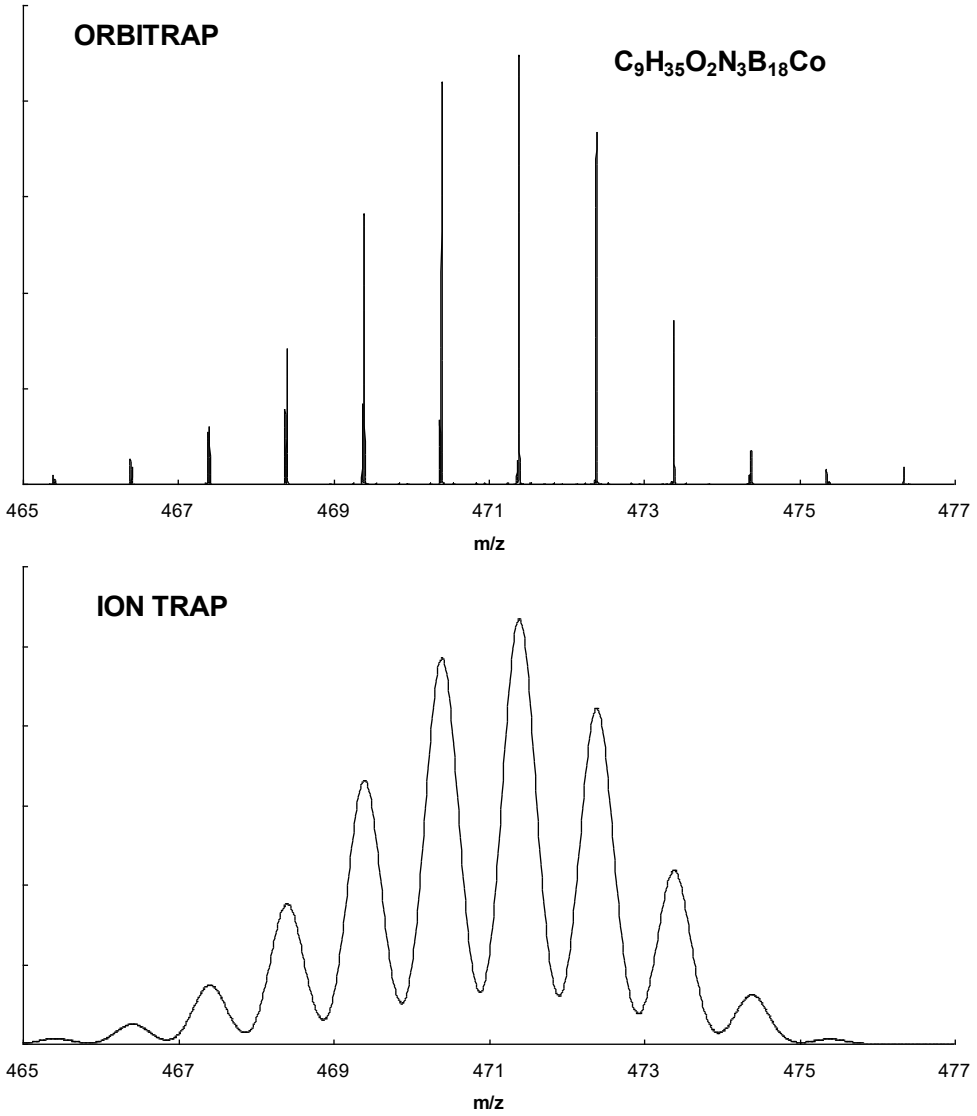






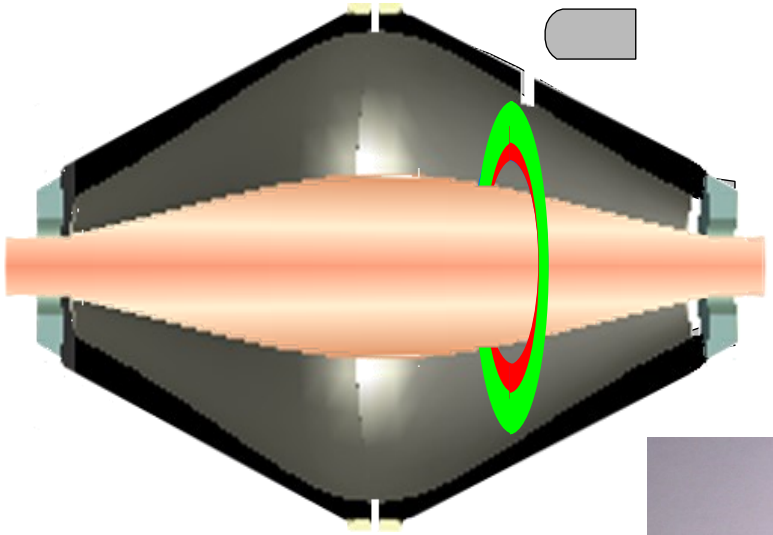
Resolution

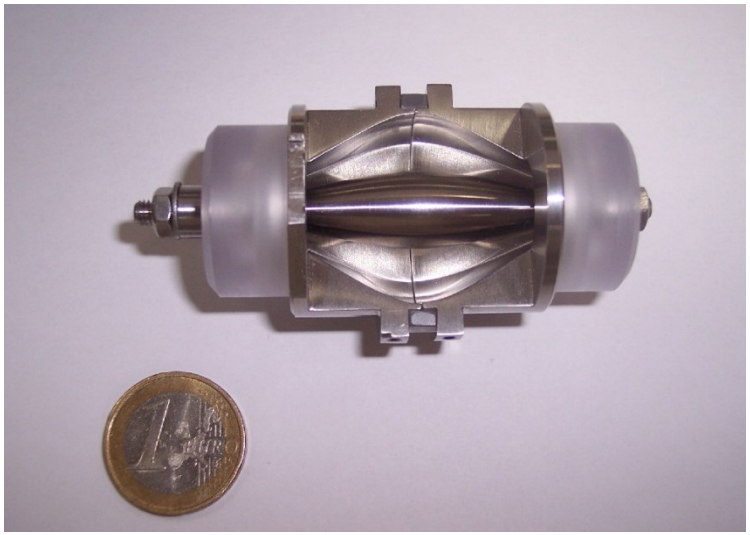
RESOLUTION



ThermoFisher SCIENTIFIC

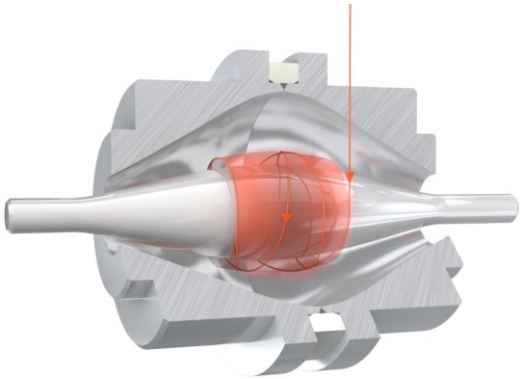
MS – Orbitrap

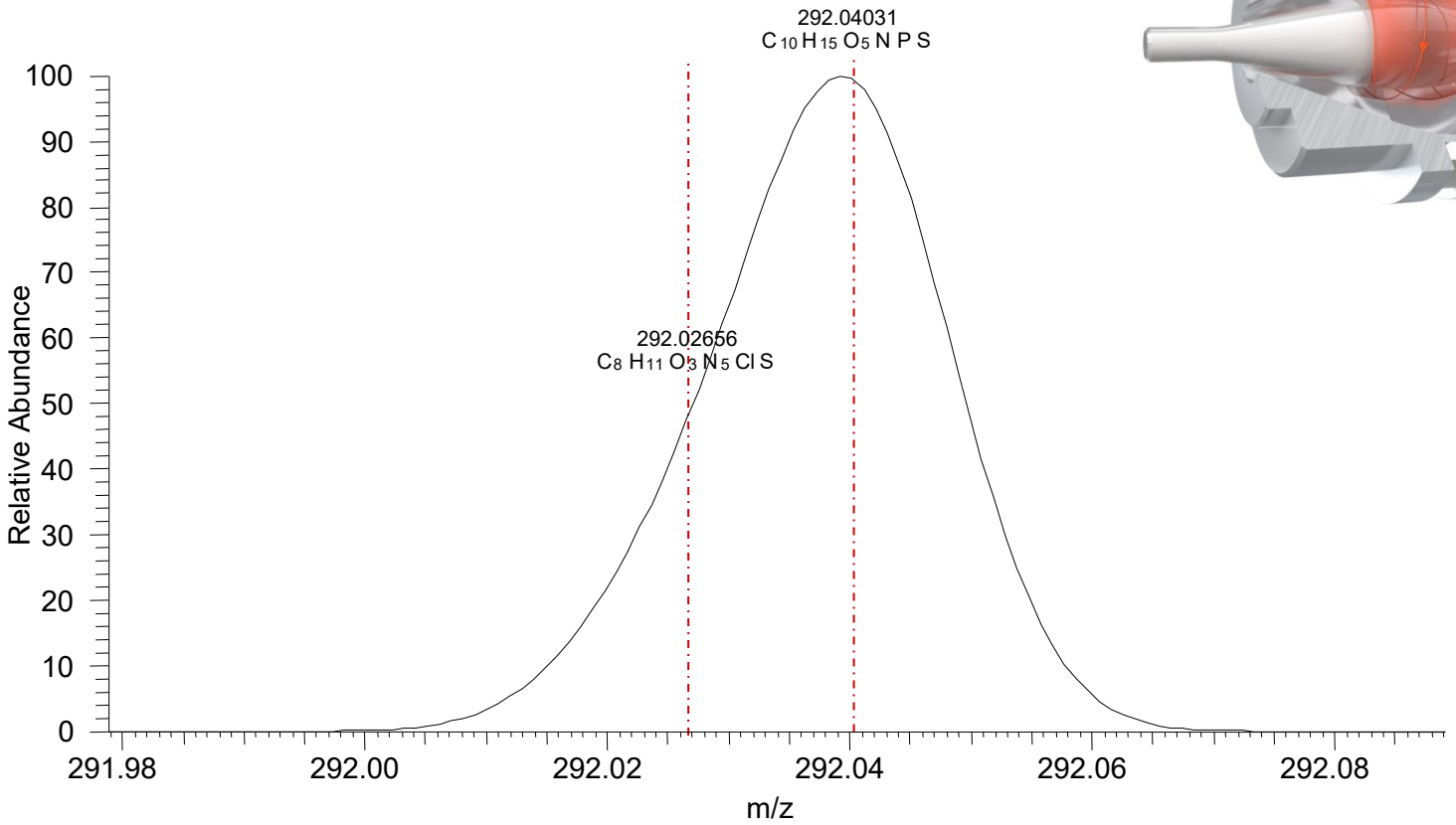




Resolution

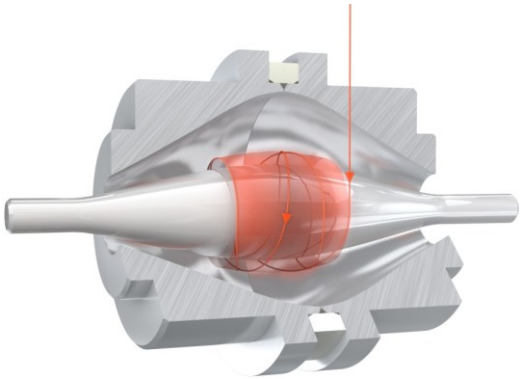
15 000

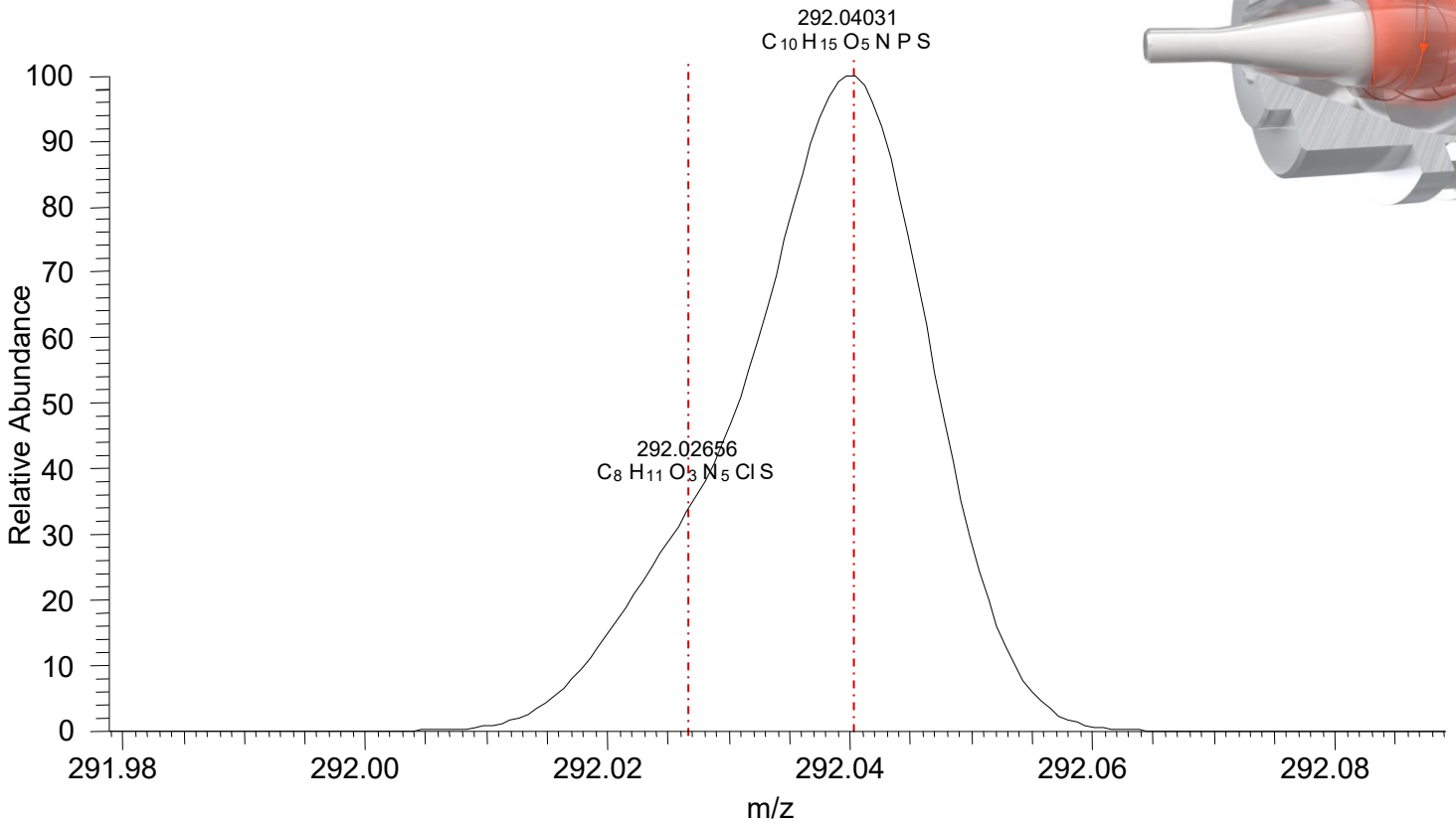




Resolution

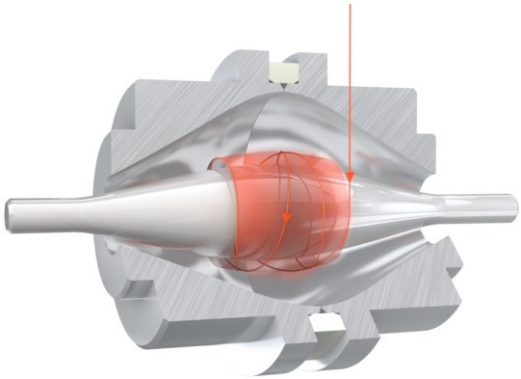
20 000

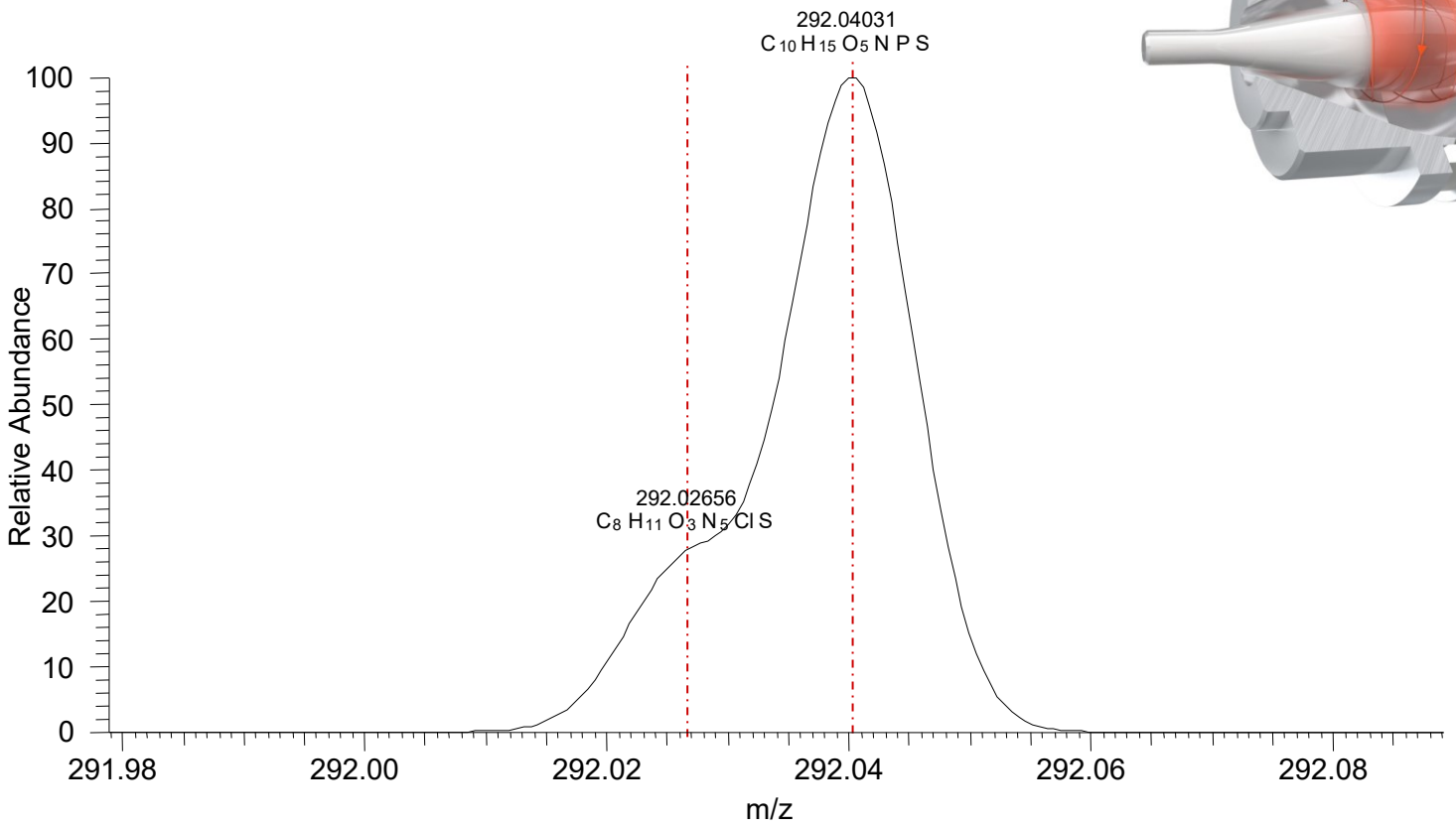




Resolution

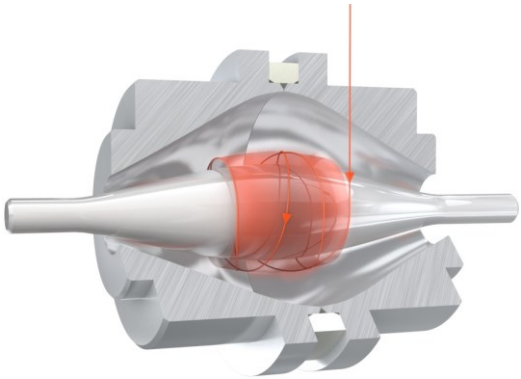
25 000

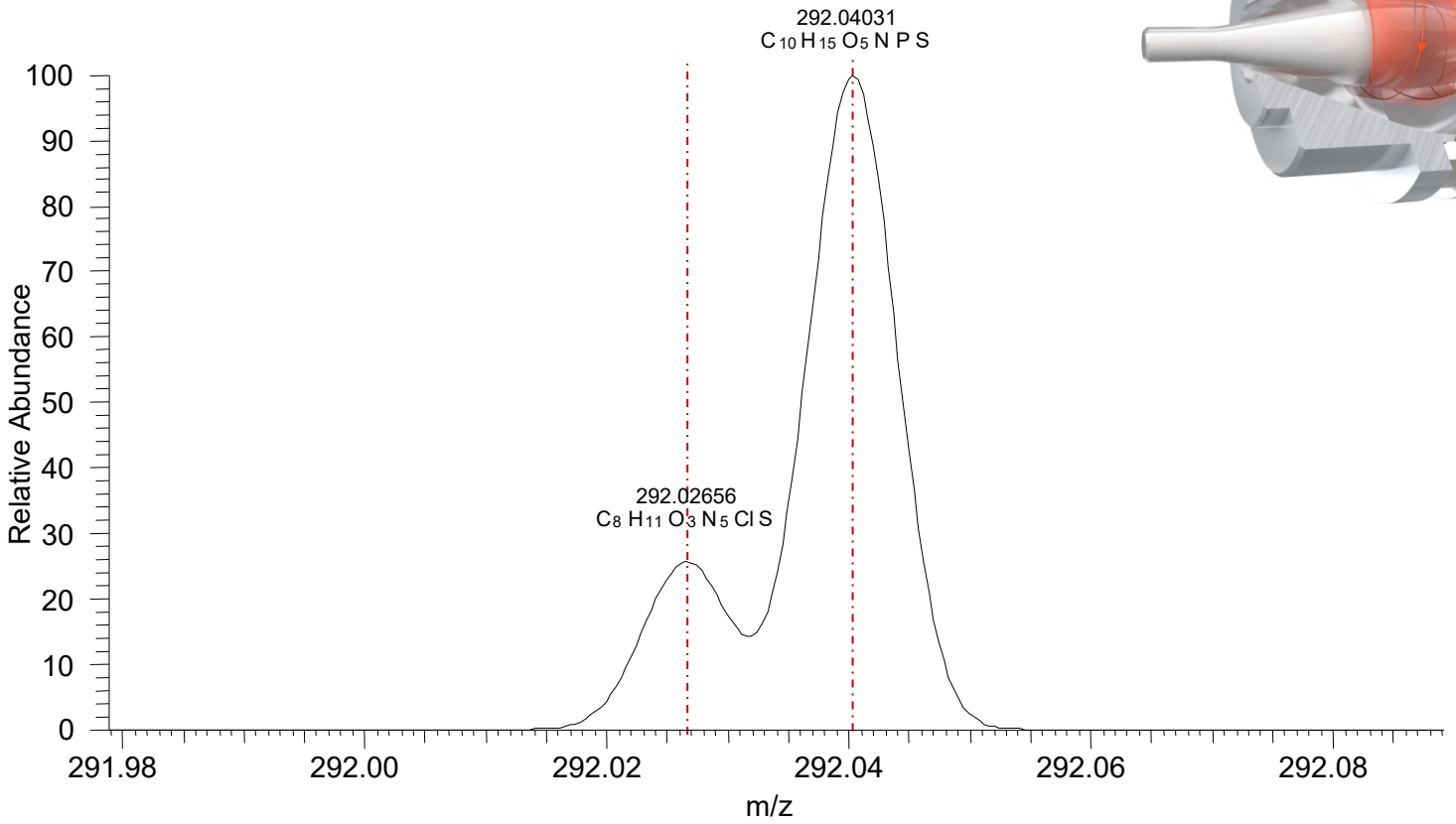




Resolution

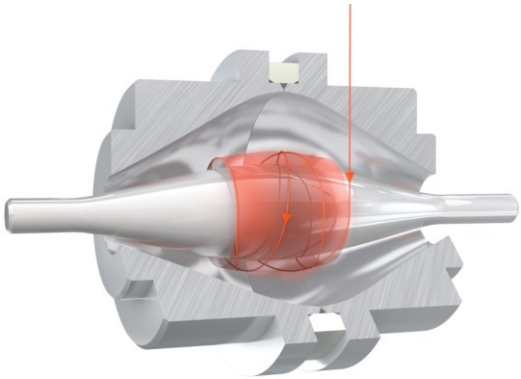
35 000

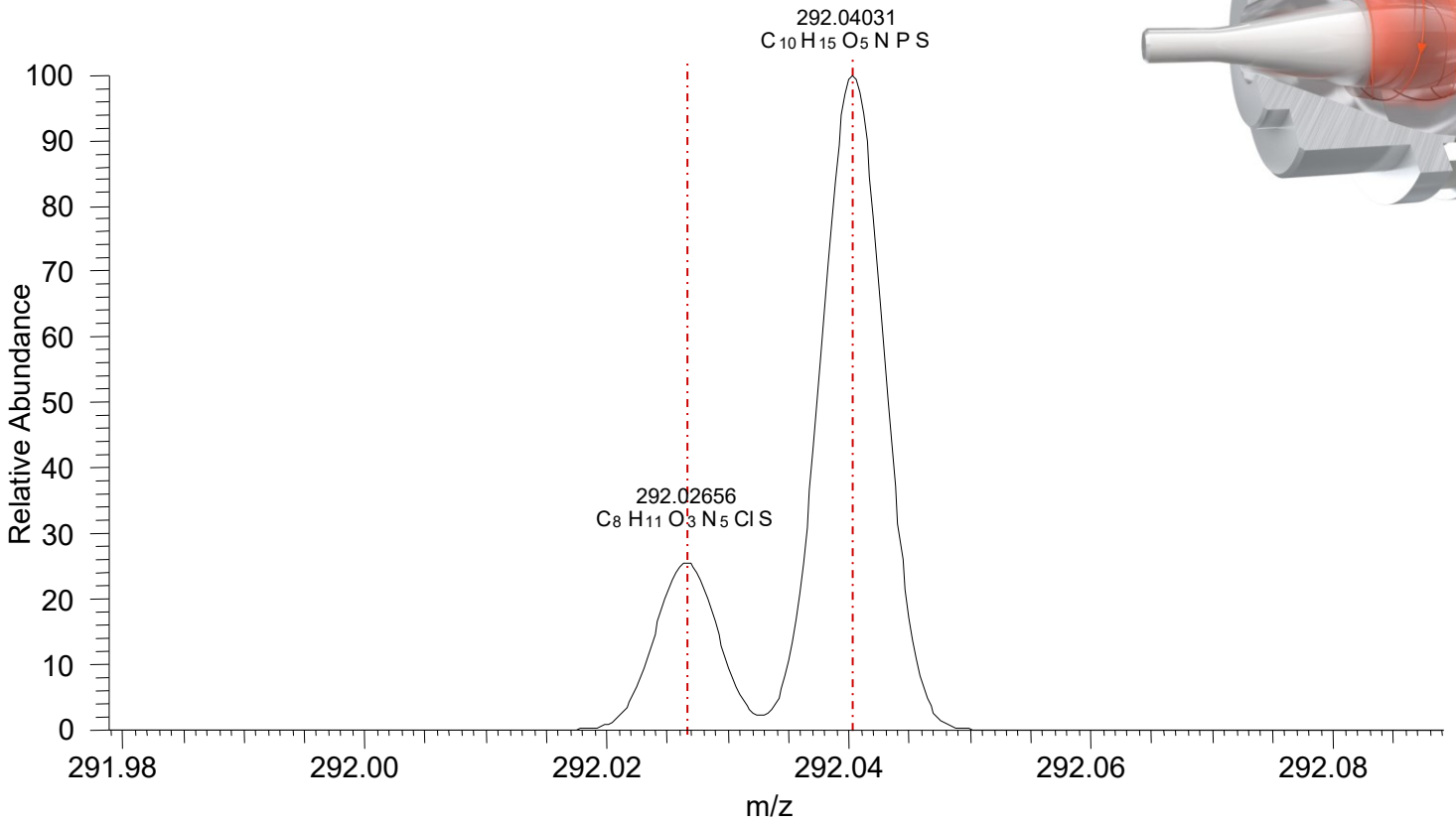




Resolution

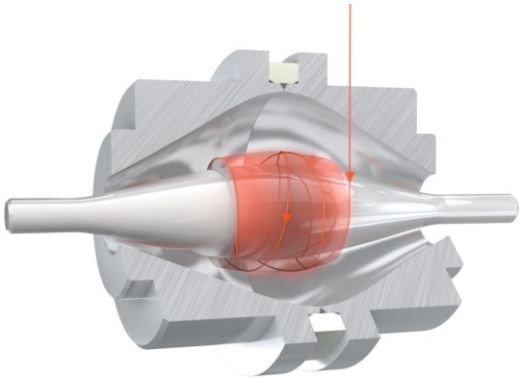
50 000

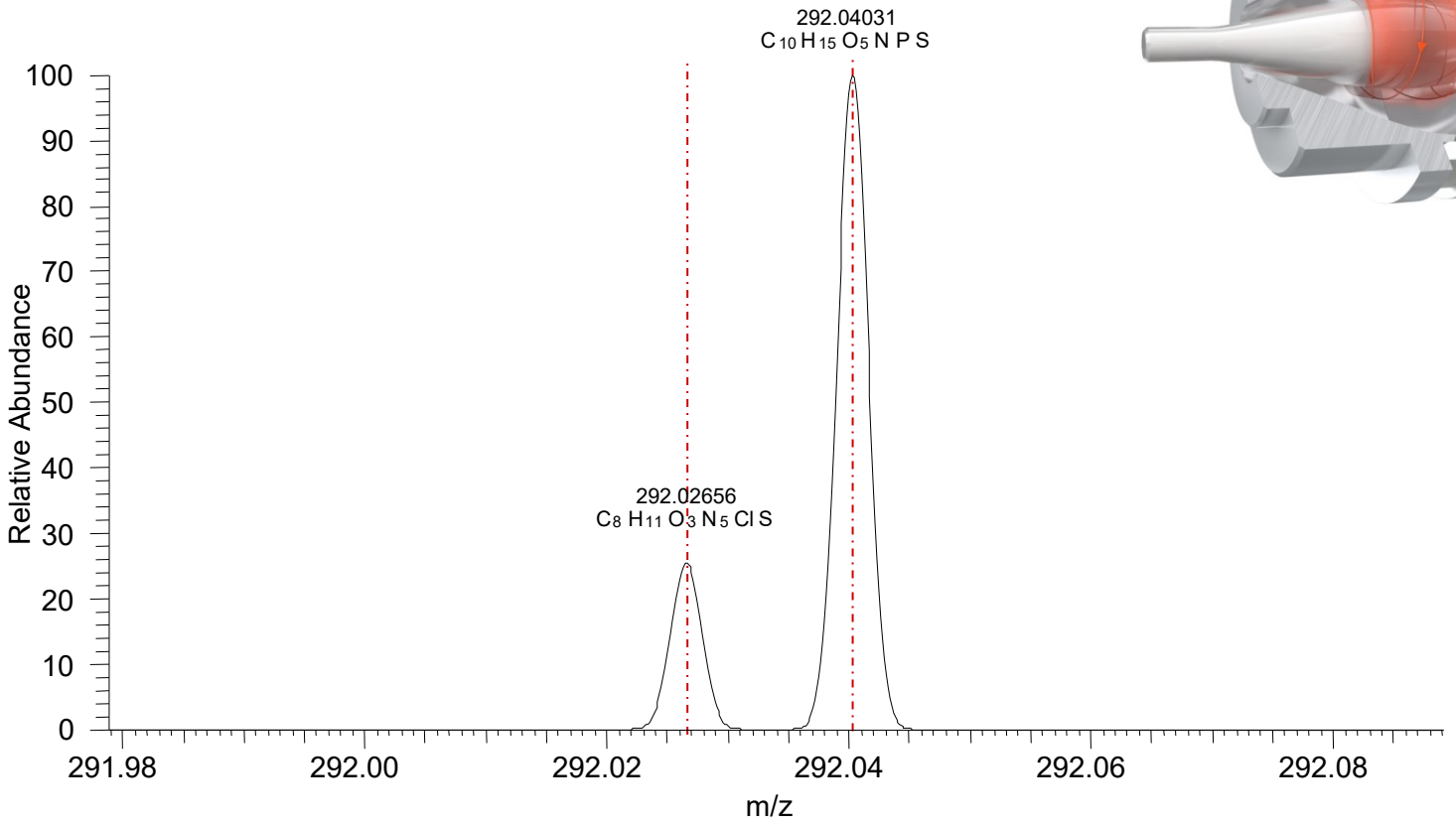




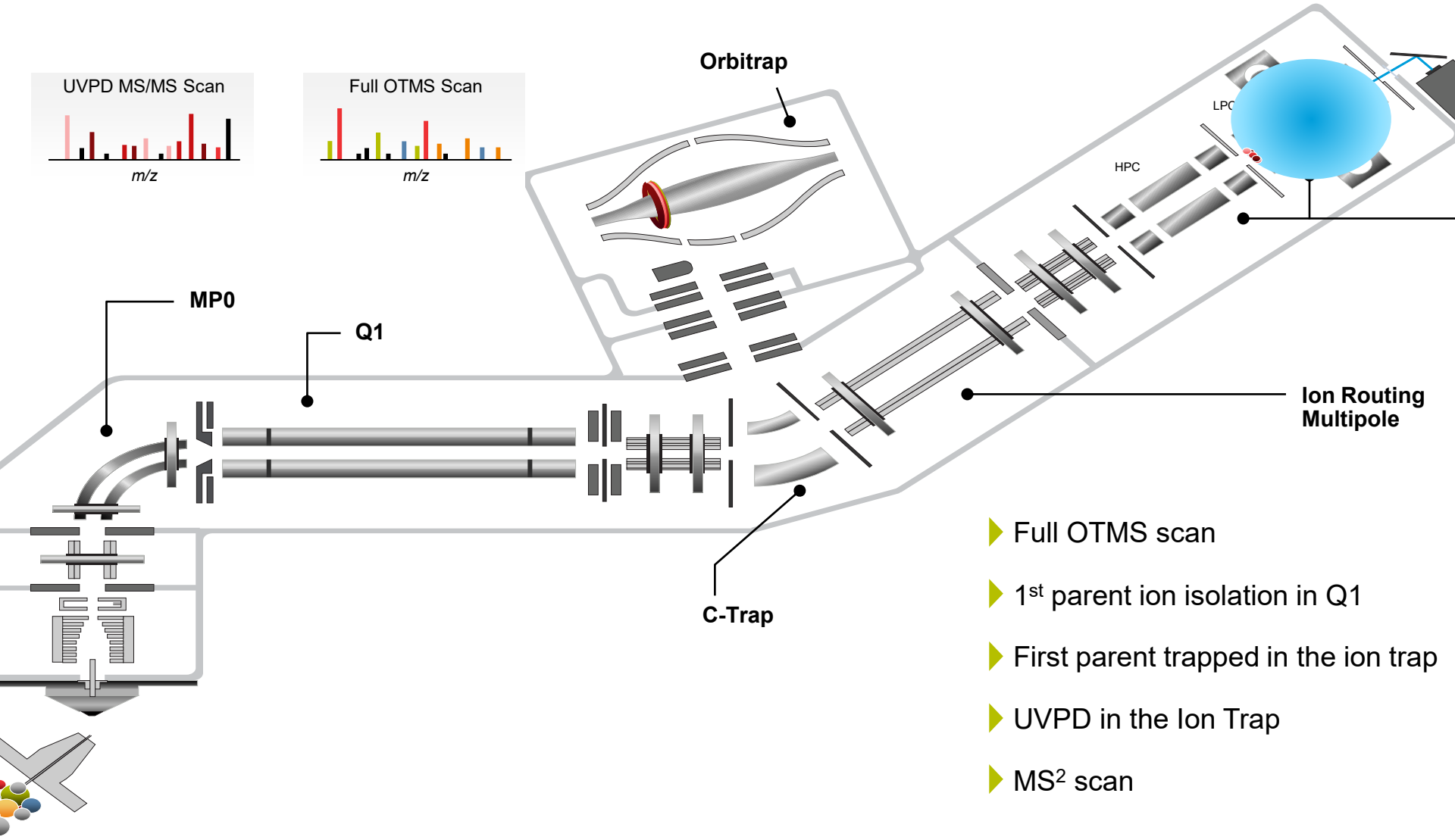
Resolution

100 000



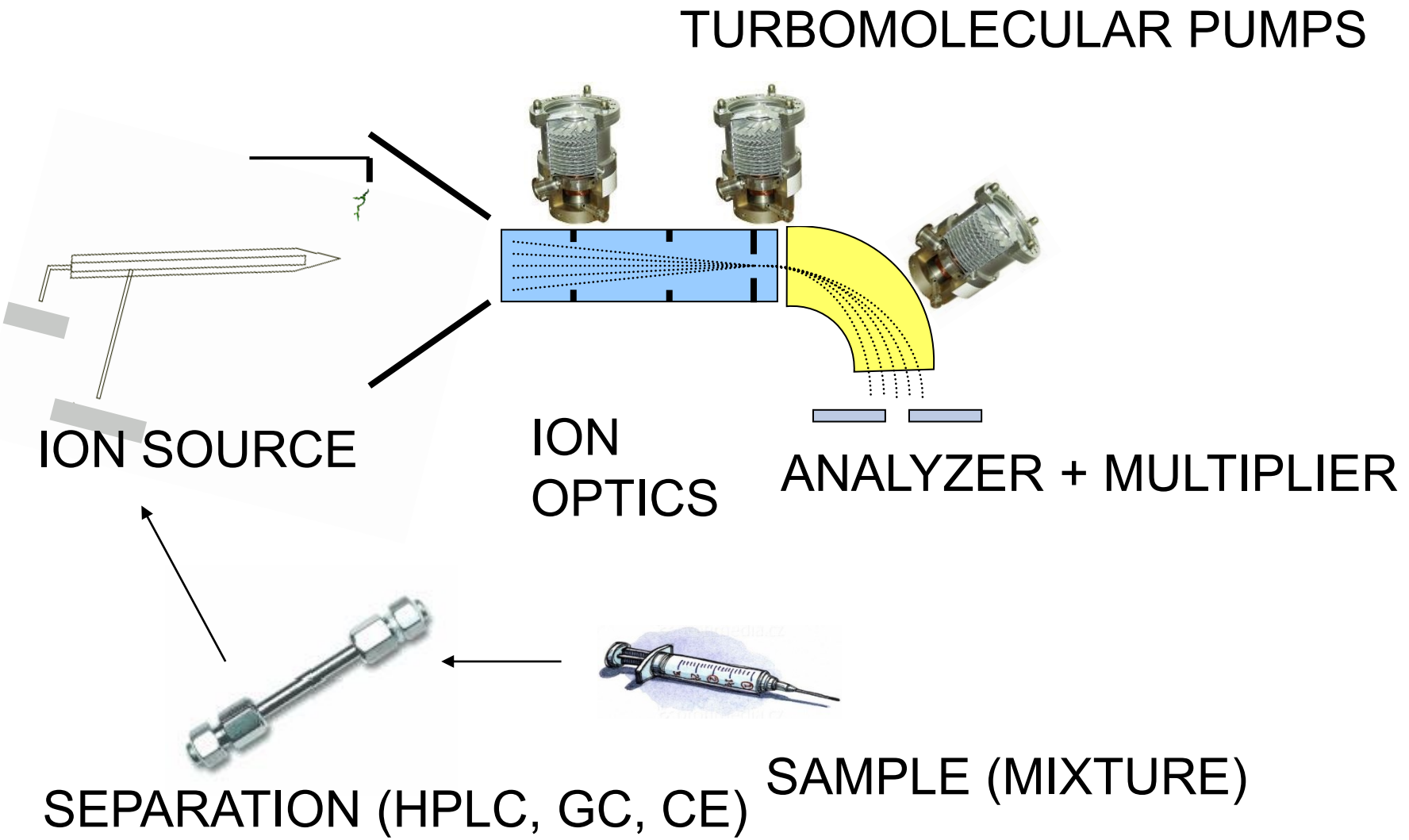


MS – Orbitrap

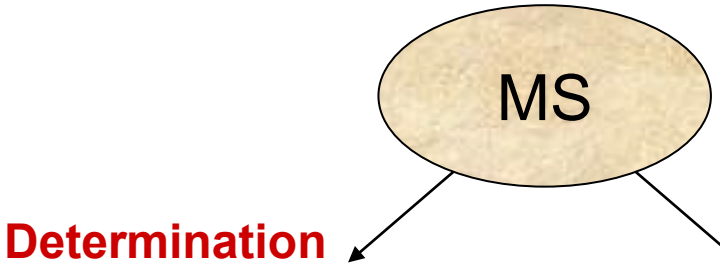


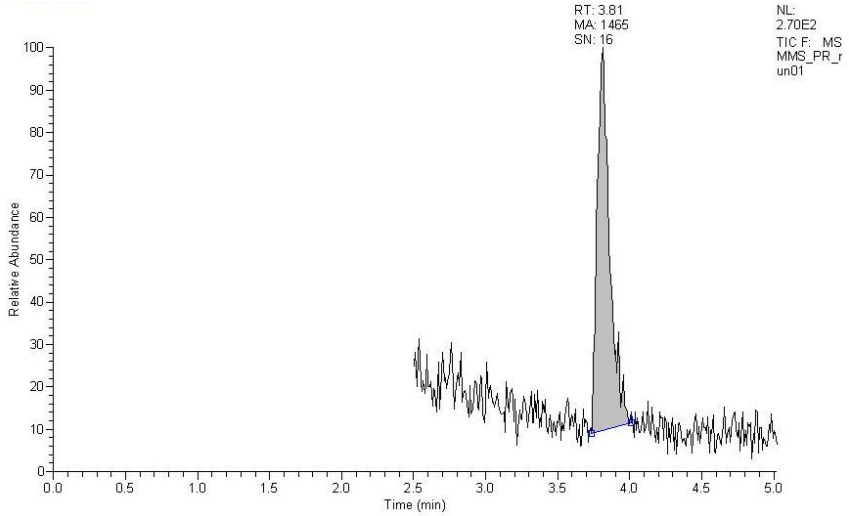
- Full OTMS scan
- 1st parent ion isolation in Q1
- First parent trapped in the ion trap
- UVPD in the Ion Trap
- MS^2 scan

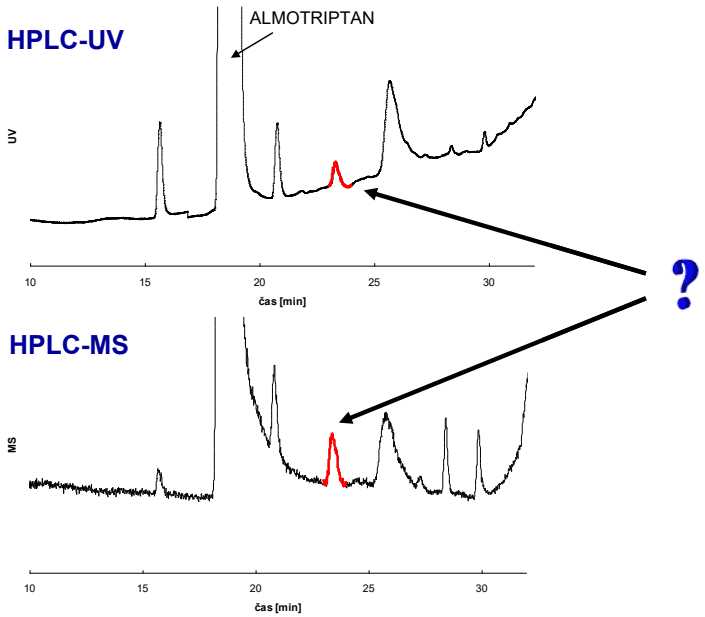
Hyphenated techniques

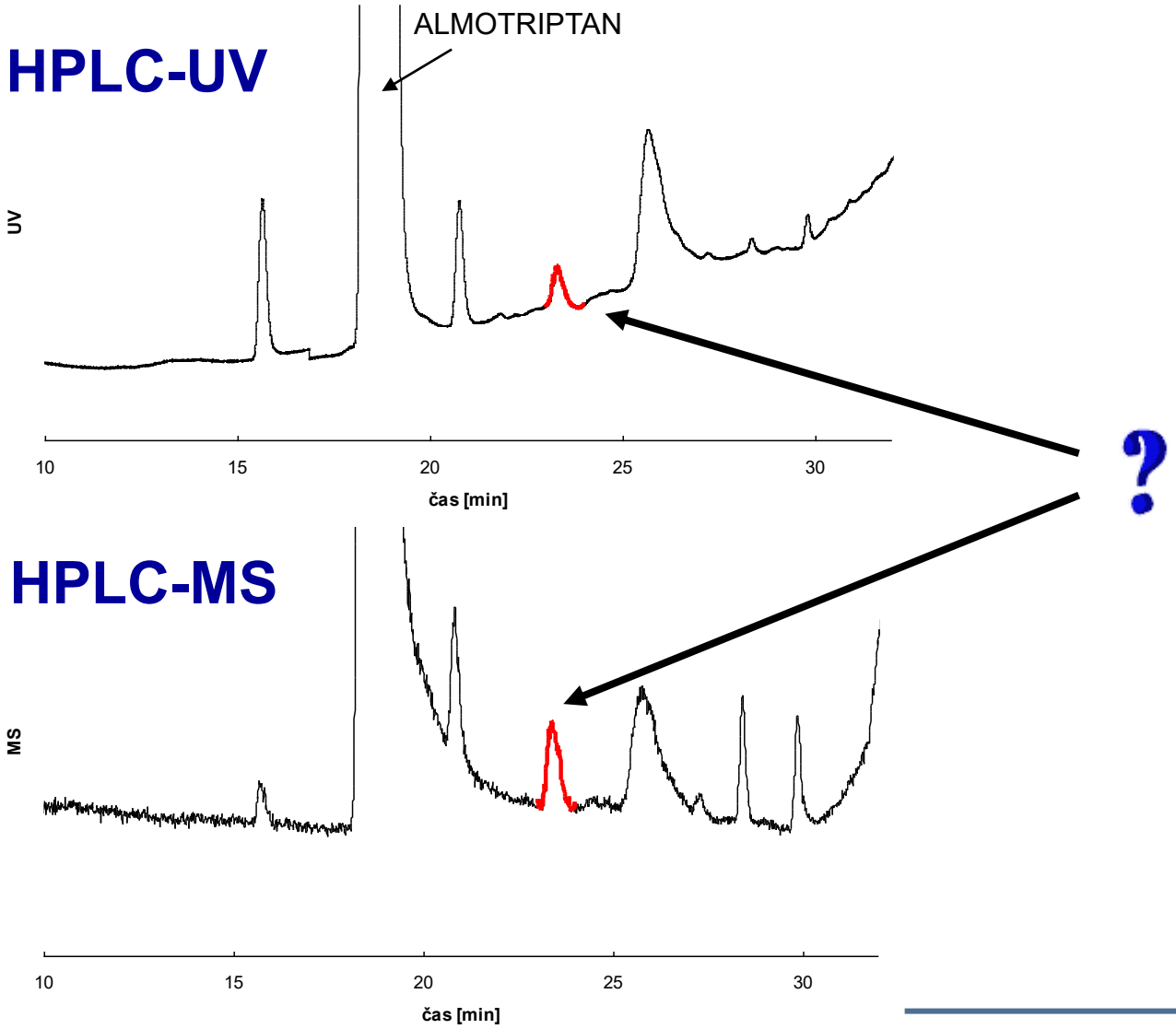


Hyphenated techniques

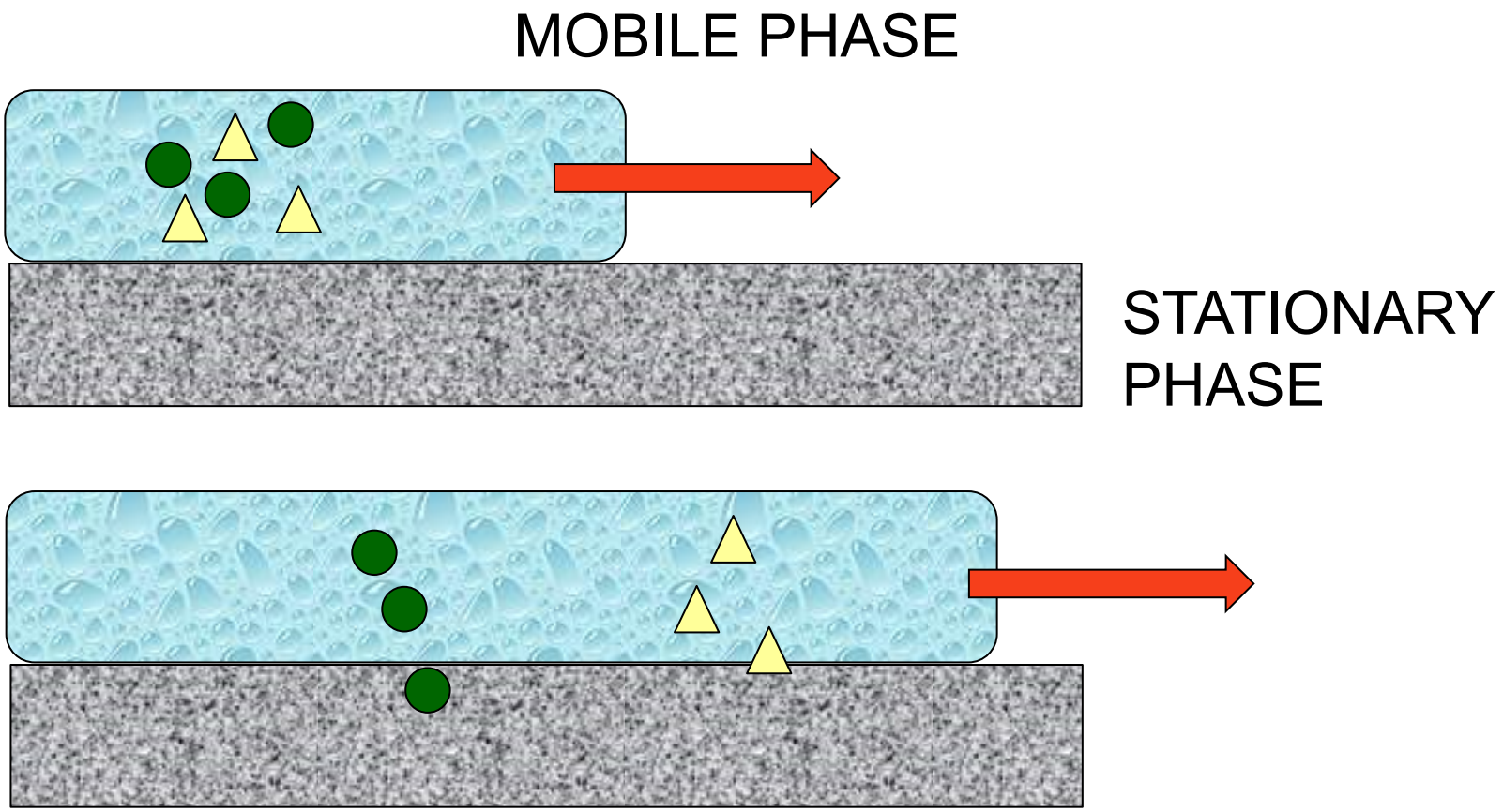






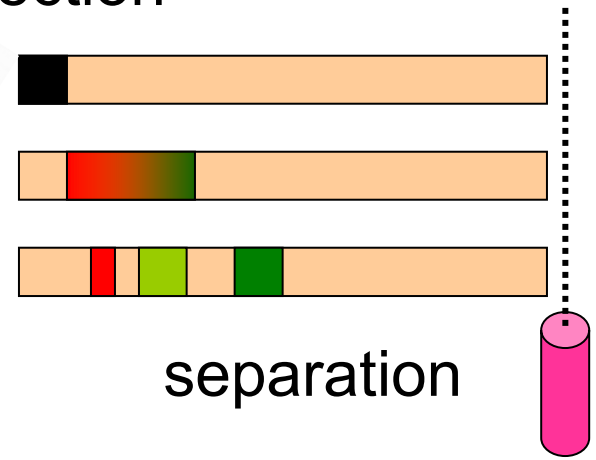


Chromatography

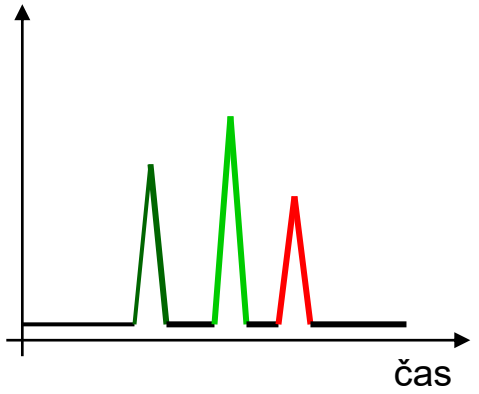


GC: gas chromatography

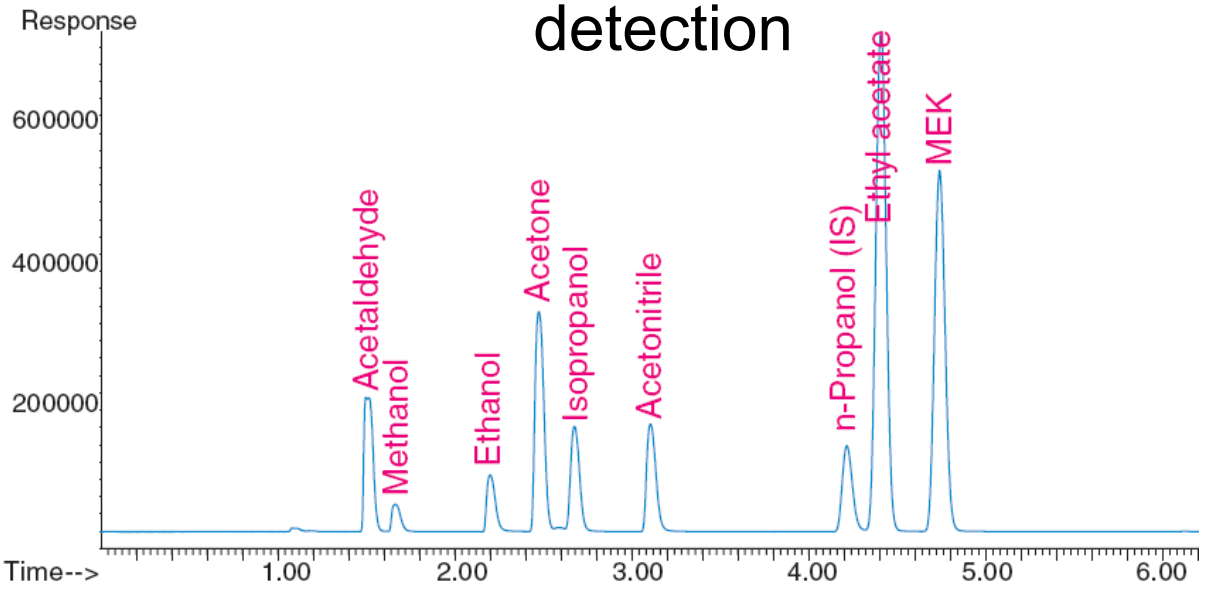
injection

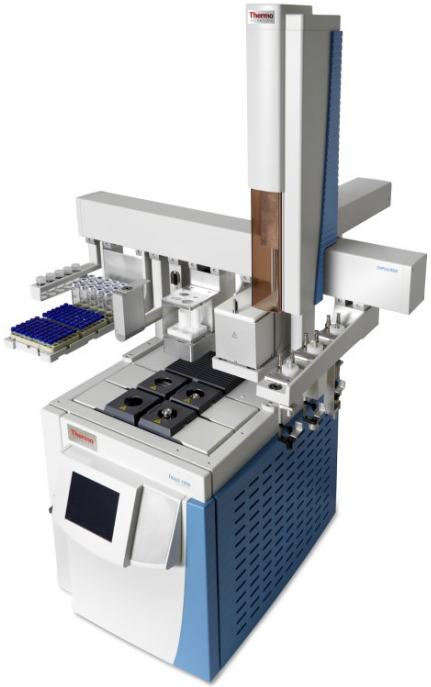


separation

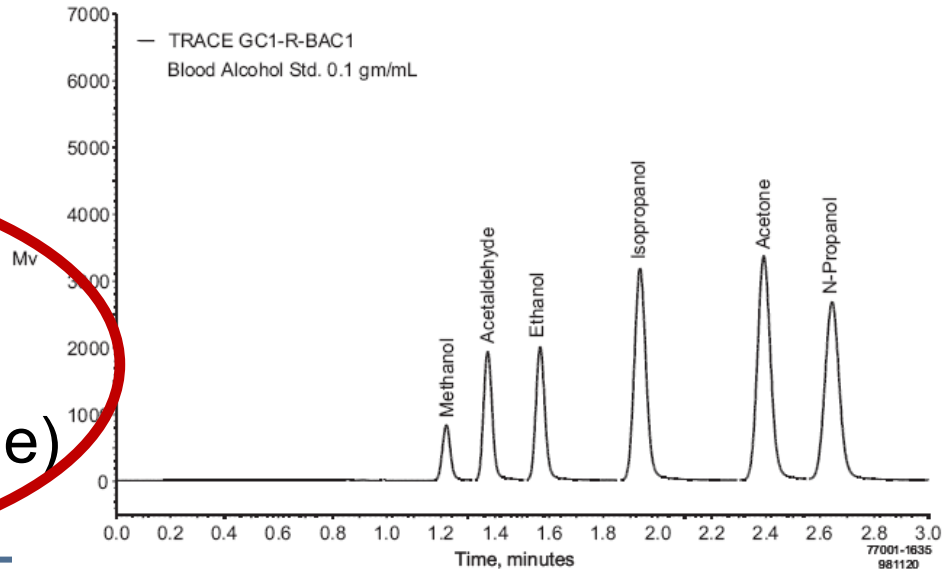


detection

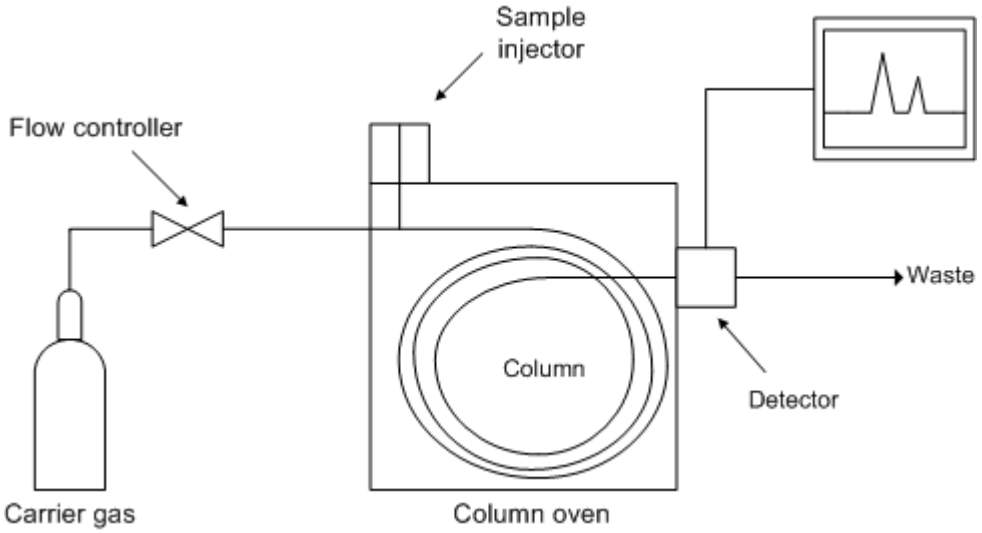




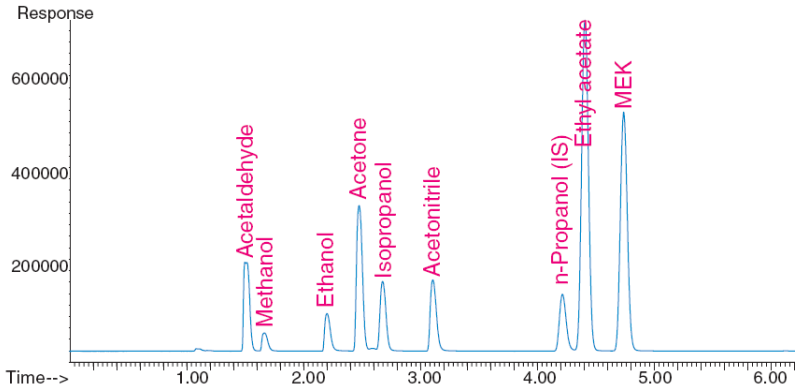
Determination of alcohol in blood (headspace technique)



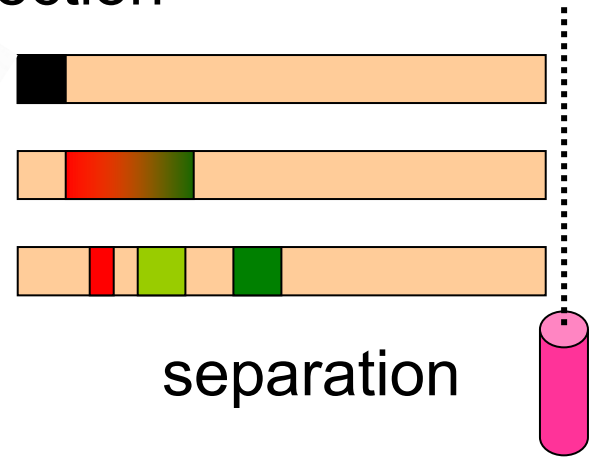
GC-MS: gas chromatography – mass spectrometry



GC-MS: gas chromatography – mass spectrometry

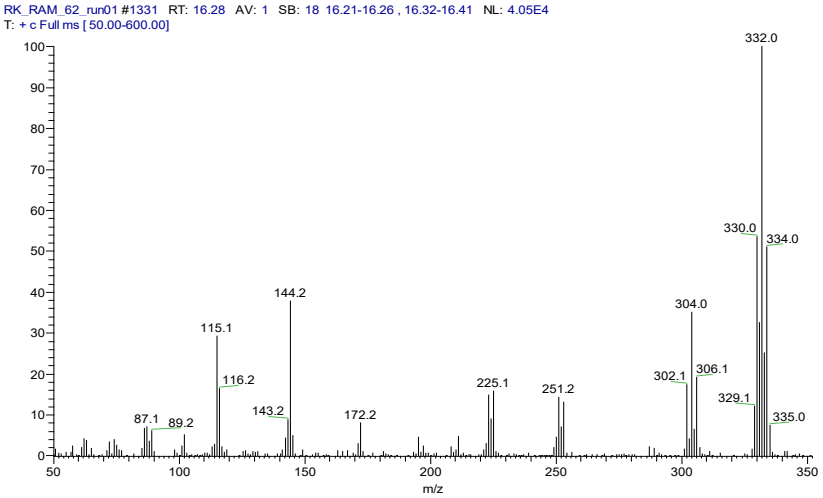


injection



separation

detection



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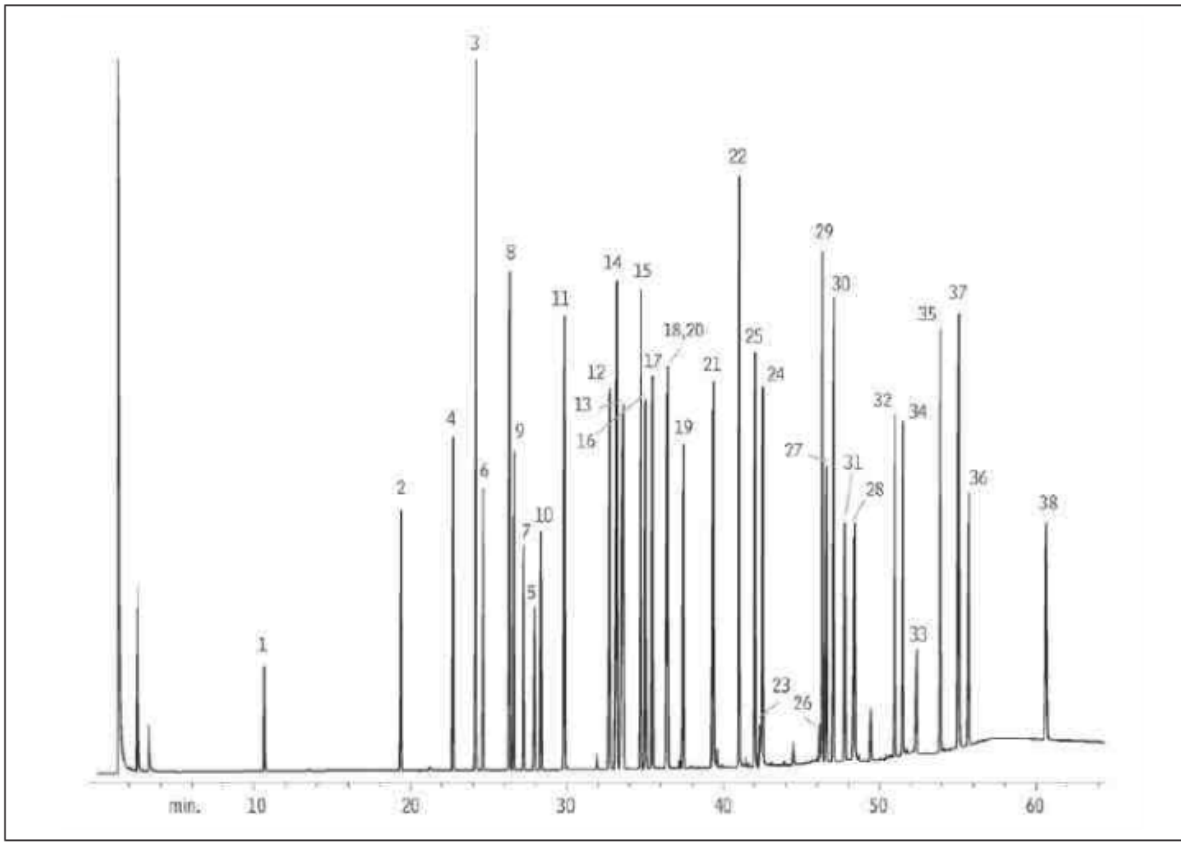
Underivatized Mixed Basic Drugs

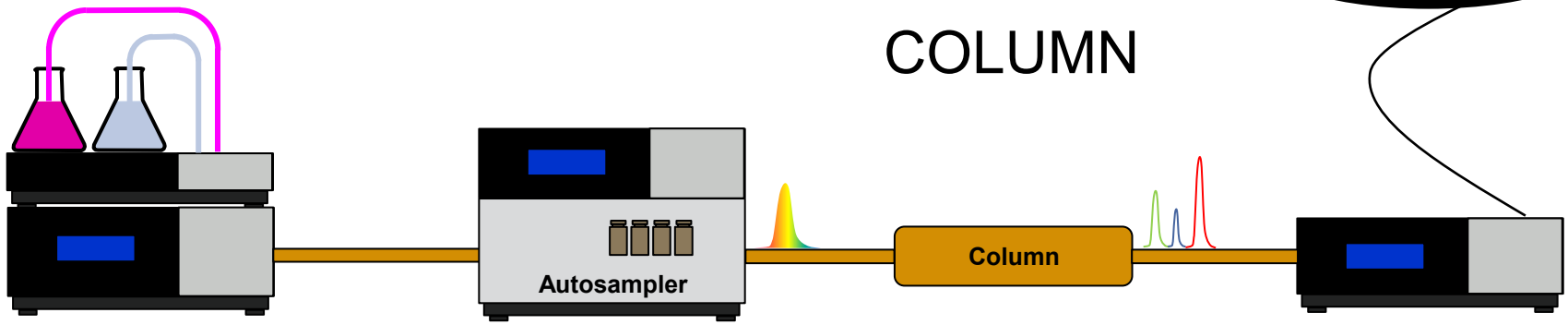
Column:	TG-35MS 30m x 0.25mm x 0.25µm
Part Number:	26094-1420
Temperature:	100°C to 325°C at 4°C/minute (10 minute hold)
Detector Type:	FID
Carrier Gas:	He
Flow Rate:	30cm/sec
Injection Volume:	1.0 µL
Injection Mode:	Split (50:1), 250°C

1. nicotine
2. benzocaine
3. cotinine
4. meperidine
5. caffeine
6. benzphetamine
7. ketamine
8. diphenhydramine
9. lidocaine
10. phenyltoloxamine
11. tripelennamine
12. phenothiazine
13. dextromethorphan
14. methadone
15. amitriptyline
16. trimipramine
17. tetracaine
18. pyrilamine
19. medazepam
20. bupivacaine
21. scopolamine
22. codeine
23. morphine
24. diazepam
25. chlorpromazine
26. temazepam
27. flunitrazepam
28. bromazepam
29. prazepam
30. acetopromazine
31. flurazepam
32. papaverine
33. clonazepam
34. haloperidol
35. alprazolam
36. triazolam
37. thioridazine
38. trazodone



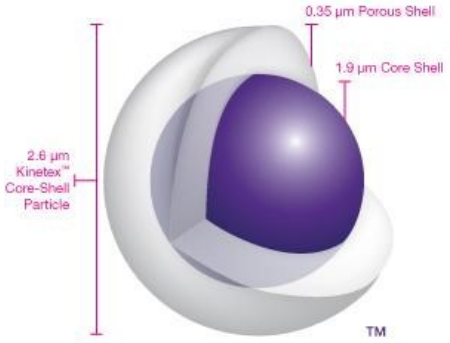
ThermoFisher SCIENTIFIC

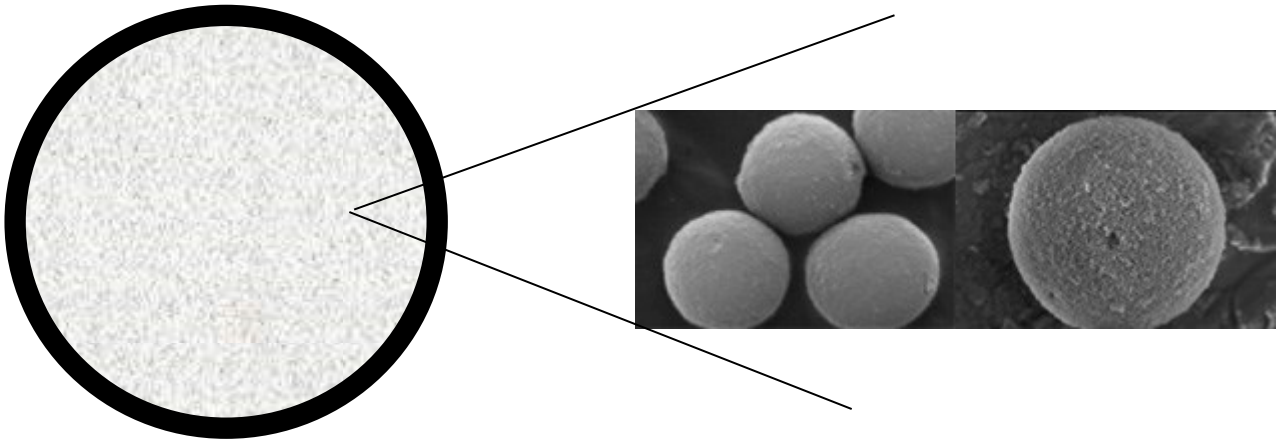
Configuration HPLC

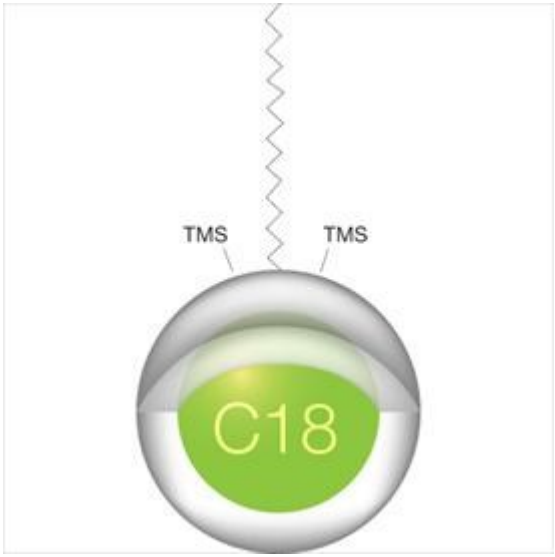


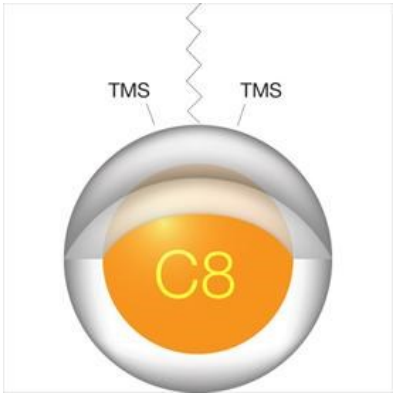
HPLC

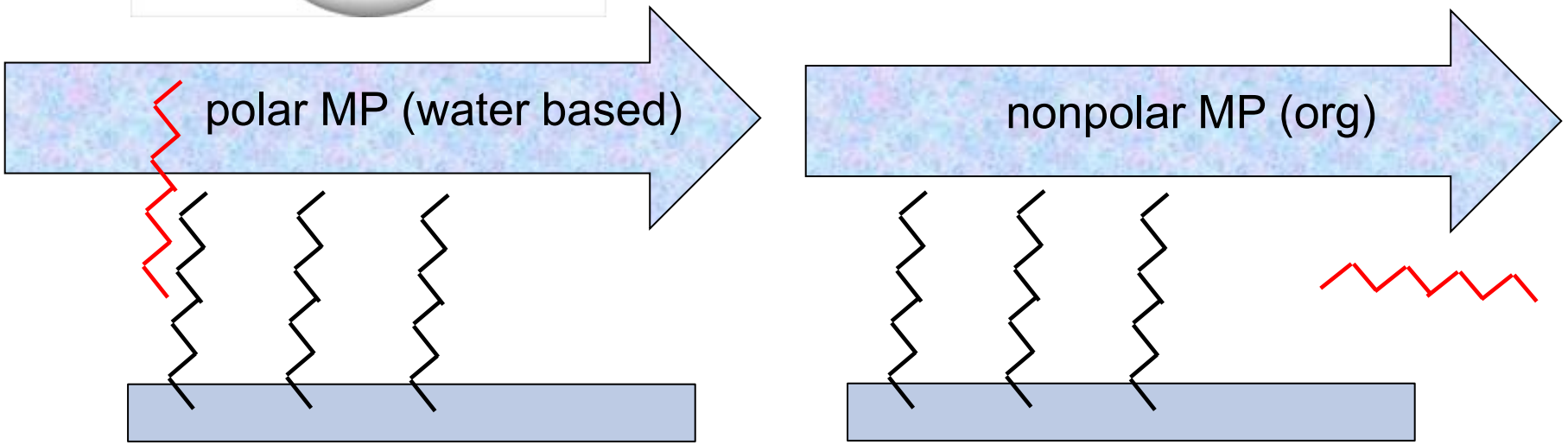
250 mm x 4.6 mm x 5 um



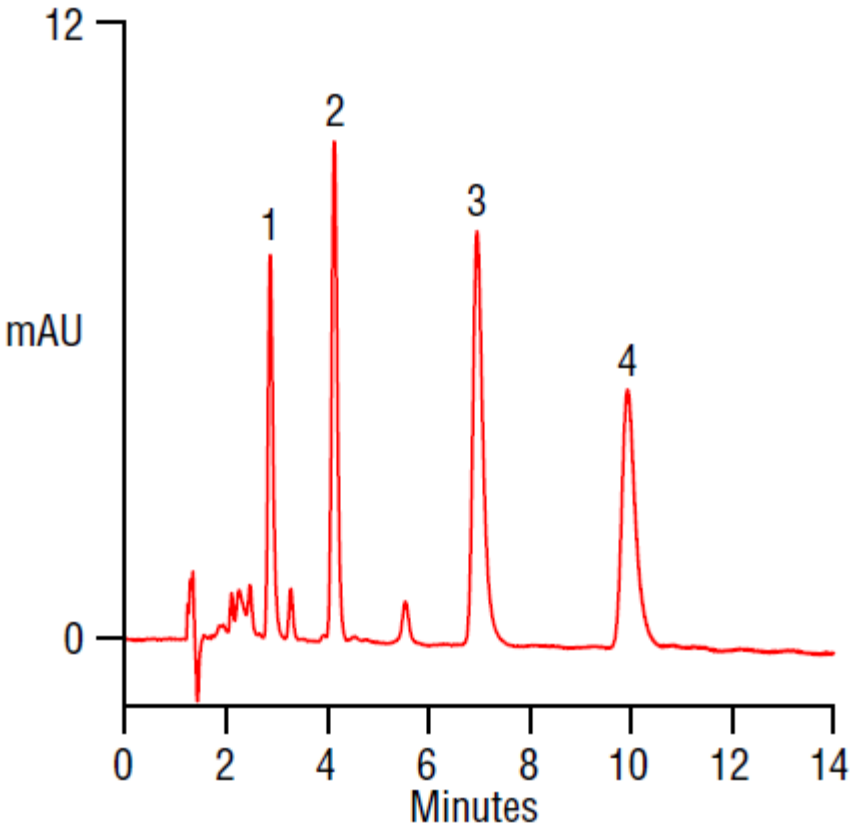




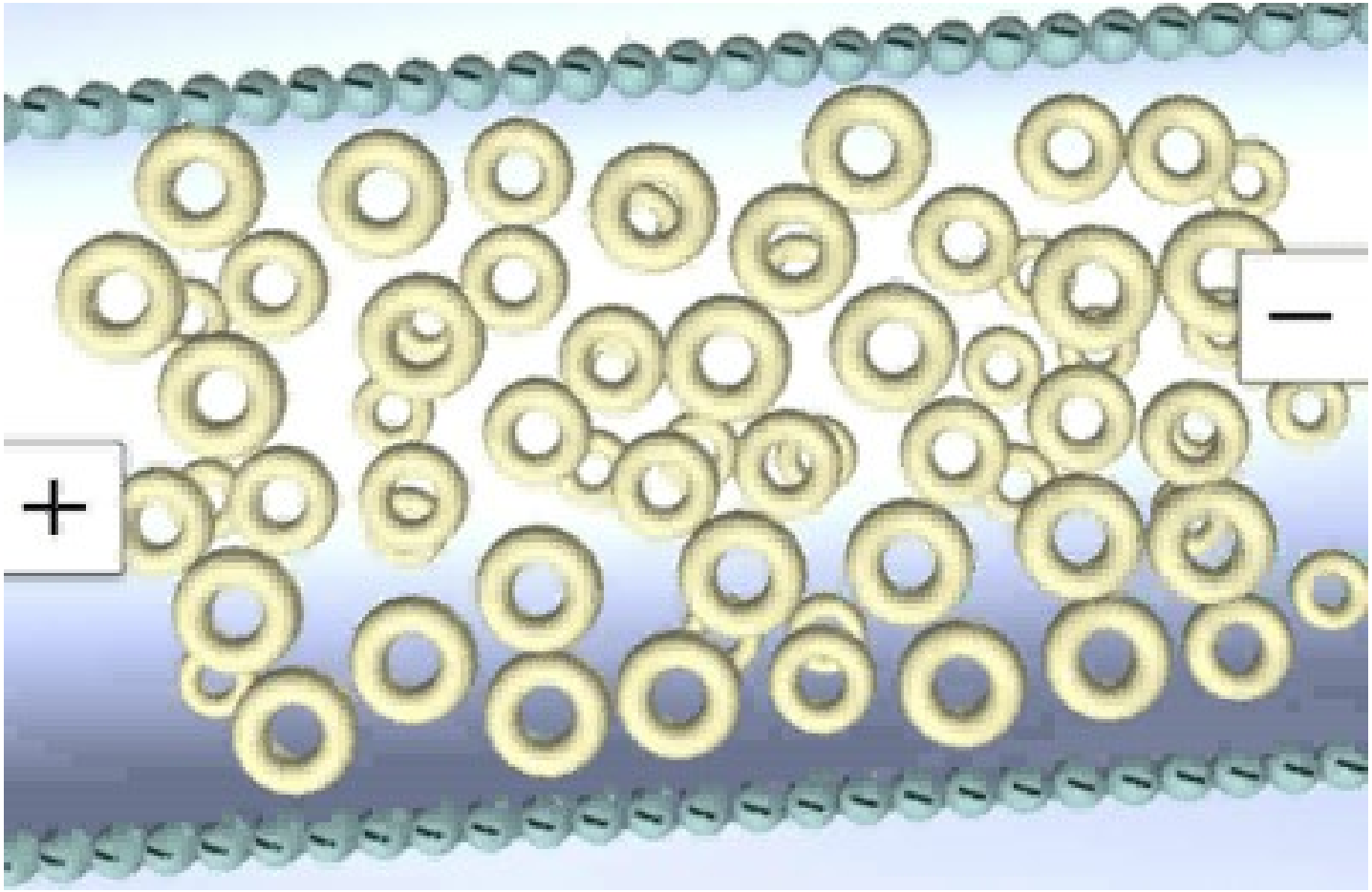




Isocratic Resolution of Antihistamines and Their Impurities on Acclaim® 120 C18

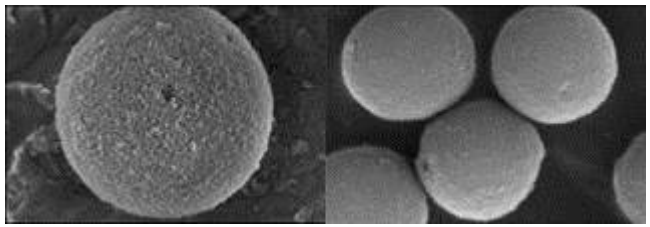


Column:	Acclaim 120 C18, 5 µm
Dimensions:	4.6 × 150 mm
Mobile Phase:	(A) 50 mM sodium acetate (B) Methanol
Isocratic:	(A) 20%, (B) 80%
Temperature:	25 °C
Detection:	UV, 249 nm
Peaks:	1. Thenyldiamine HCl 2. Phenothiazine 3. Promethazine HCl 4. Pyrrobutamine phosphate

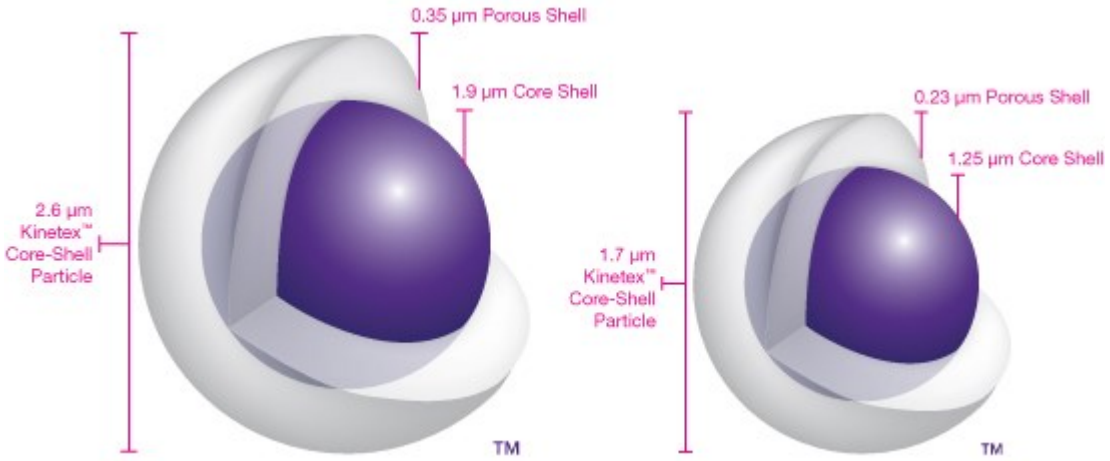


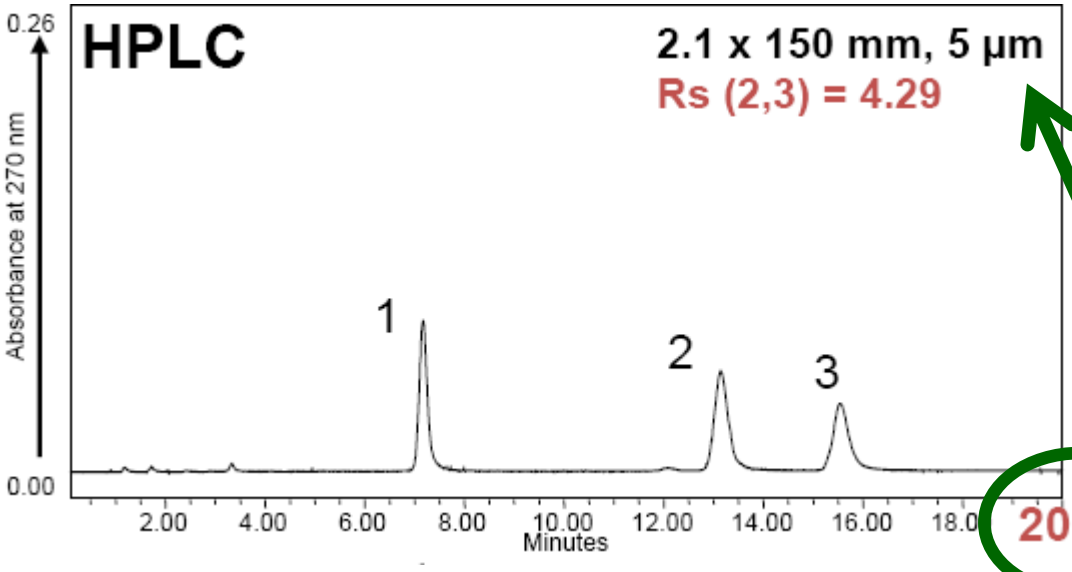
Trends: U-HPLC

Ultra-High-Performance-Liquid-Chromatography

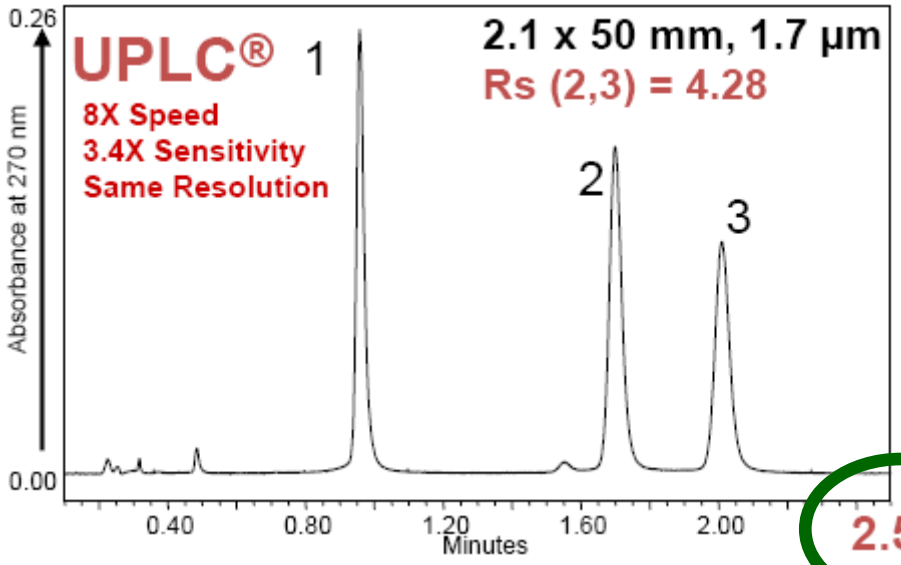


< 200 bar → > 400 bar





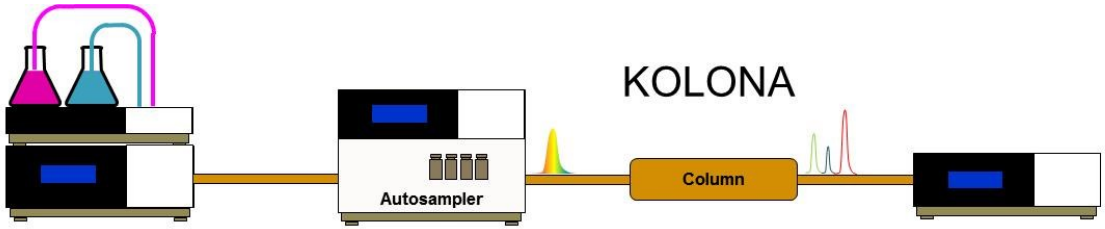
ULTRA HPLC
U-HPLC



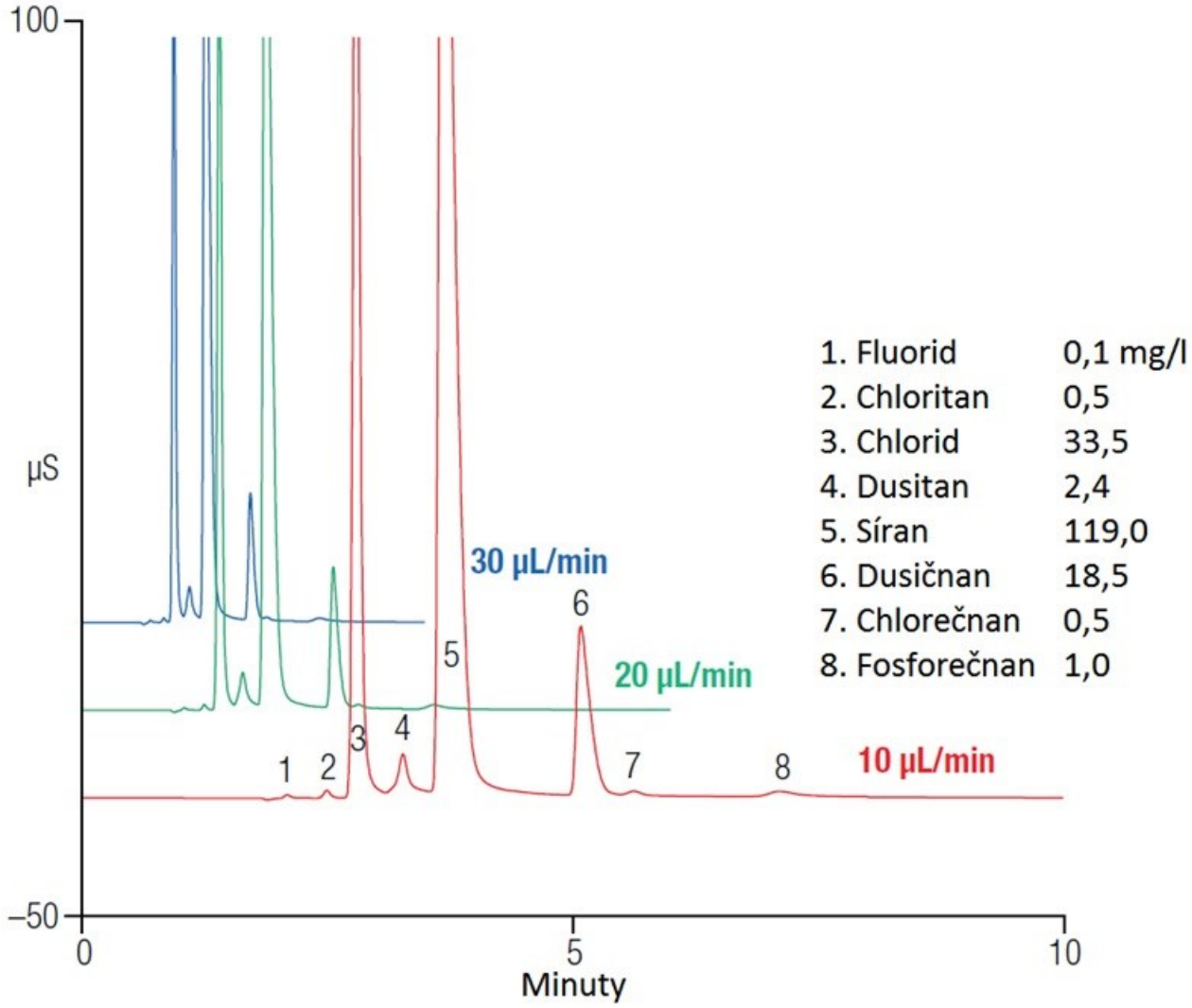
Pressure up to 1500 bar

ThermoFisher SCIENTIFIC

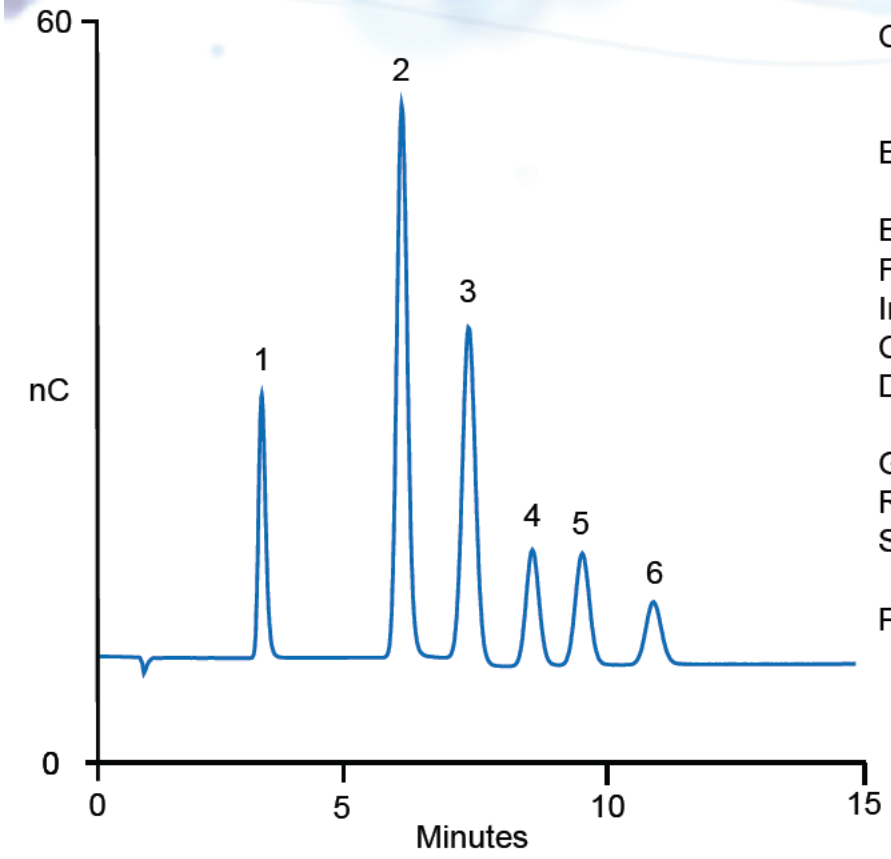
ION CHROMATOGRAPHY



PUMPA AUTOSAMPLER DETEKTOR

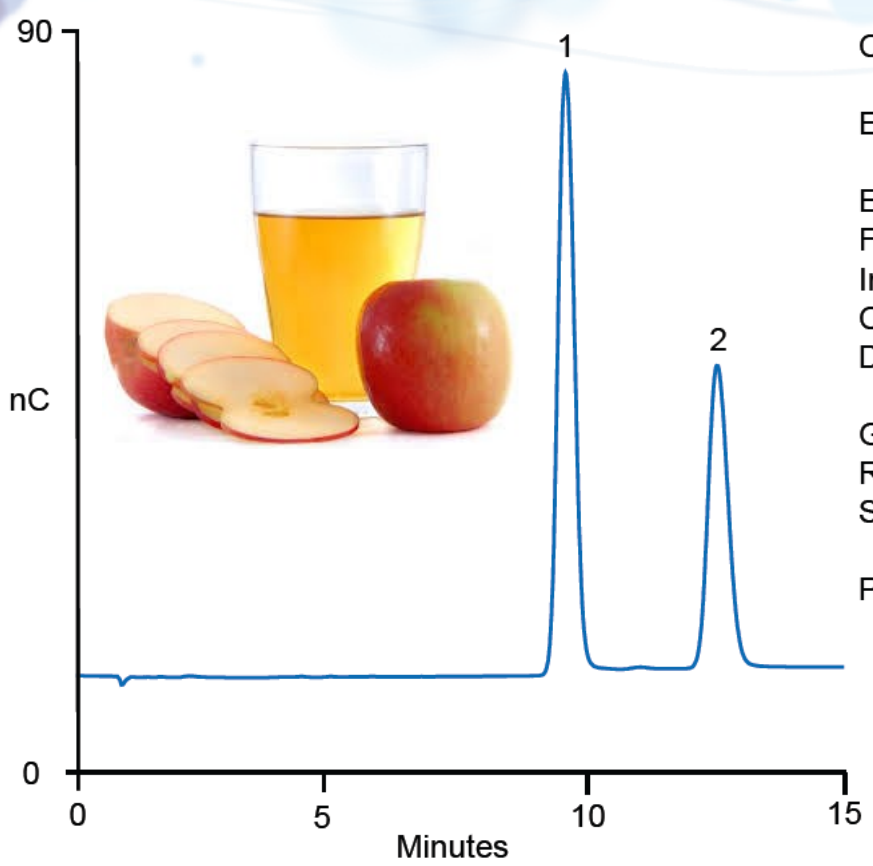


1. Fluorid	0,1 mg/l
2. Chloritan	0,5
3. Chlorid	33,5
4. Dusitan	2,4
5. Síran	119,0
6. Dusičnan	18,5
7. Chlorečnan	0,5
8. Fosforečnan	1,0



Column:	Thermo Scientific™ Dionex™ CarboPac™ PA20 with guard, 0.4 mm
Eluent Source:	Thermo Scientific Dionex EGC-KOH (Capillary) cartridge
Eluent:	10 mM KOH
Flow Rate:	0.008 mL/min
Inj. Volume:	0.4 µL
Column Temp.:	30 °C
Detection:	PAD, Au disposable, 4-Potential Carbohydrate waveform
Gasket:	0.001" PTFE
Ref. Electrode:	Ag/AgCl
Samples:	10 µM mixed standard

Peaks:
1. Fucose
2. Galactosamine
3. Glucosamine
4. Galactose
5. Glucose
6. Mannose



Column:	Dionex CarboPac PA20 with guard, 0.4 mm
Eluent Source:	Dionex EGC-KOH (Capillary) cartridge
Eluent:	10 mM KOH
Flow Rate:	0.008 mL/min
Inj. Volume:	0.4 µL
Column Temp.:	30 °C
Detection:	PAD, Au disposable, 4-Potential Carbohydrate waveform
Gasket:	0.001" PTFE
Ref. Electrode:	Ag/AgCl
Sample Prep.:	5000-fold dilution, degas

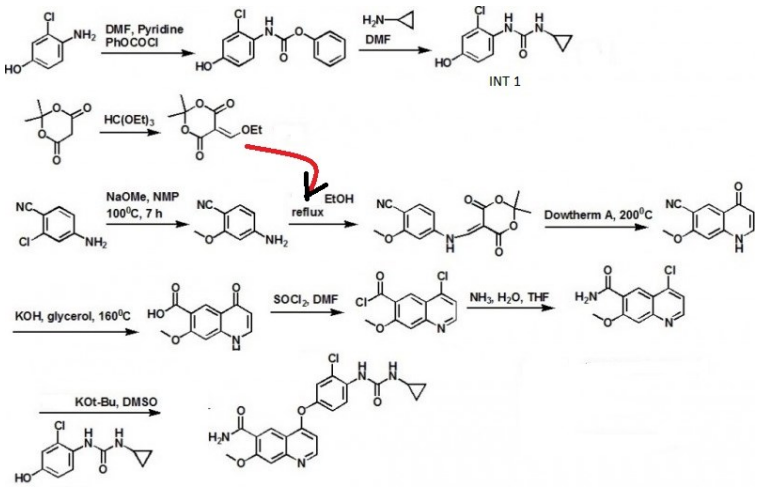
Peaks:	1. Glucose	98 µM
	2. Fructose	95

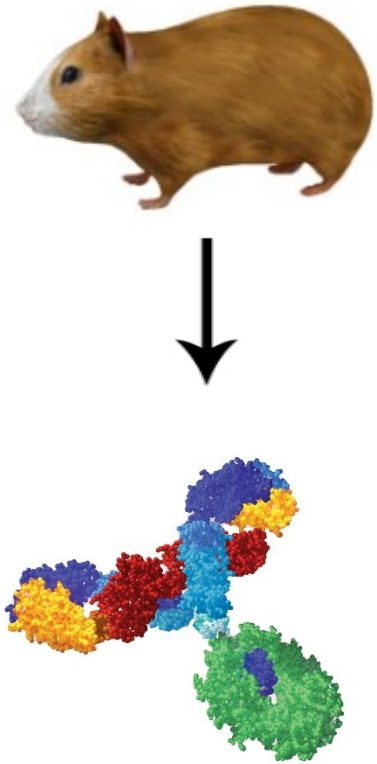

plynová chromatografie ICP-OES příprava vzorku GC temperace kapalinová chromatografie
elementární ANALÝZA elektrochemie SEA UV-VIS spektrometrie LIMS lyofilizátory
analýza povrchů separační techniky B.E.T. GC-MS koncentrátory CHNSO analýza
REOLOGIE ATOMOVÁ spektroskopie Hypercarb AAS hmotnostní SPEKTROMETRIE

2020 TRENDS

CO TO JE?

biopharmaceutical BIOLOGICAL biologic *BIOLOGICAL*
MEDICAL PRODUCTS biologické léčiva BIOPREPARÁTY
biopharma products ***biofarmaka*** biofarmaceutika **BIOLOGICAL**

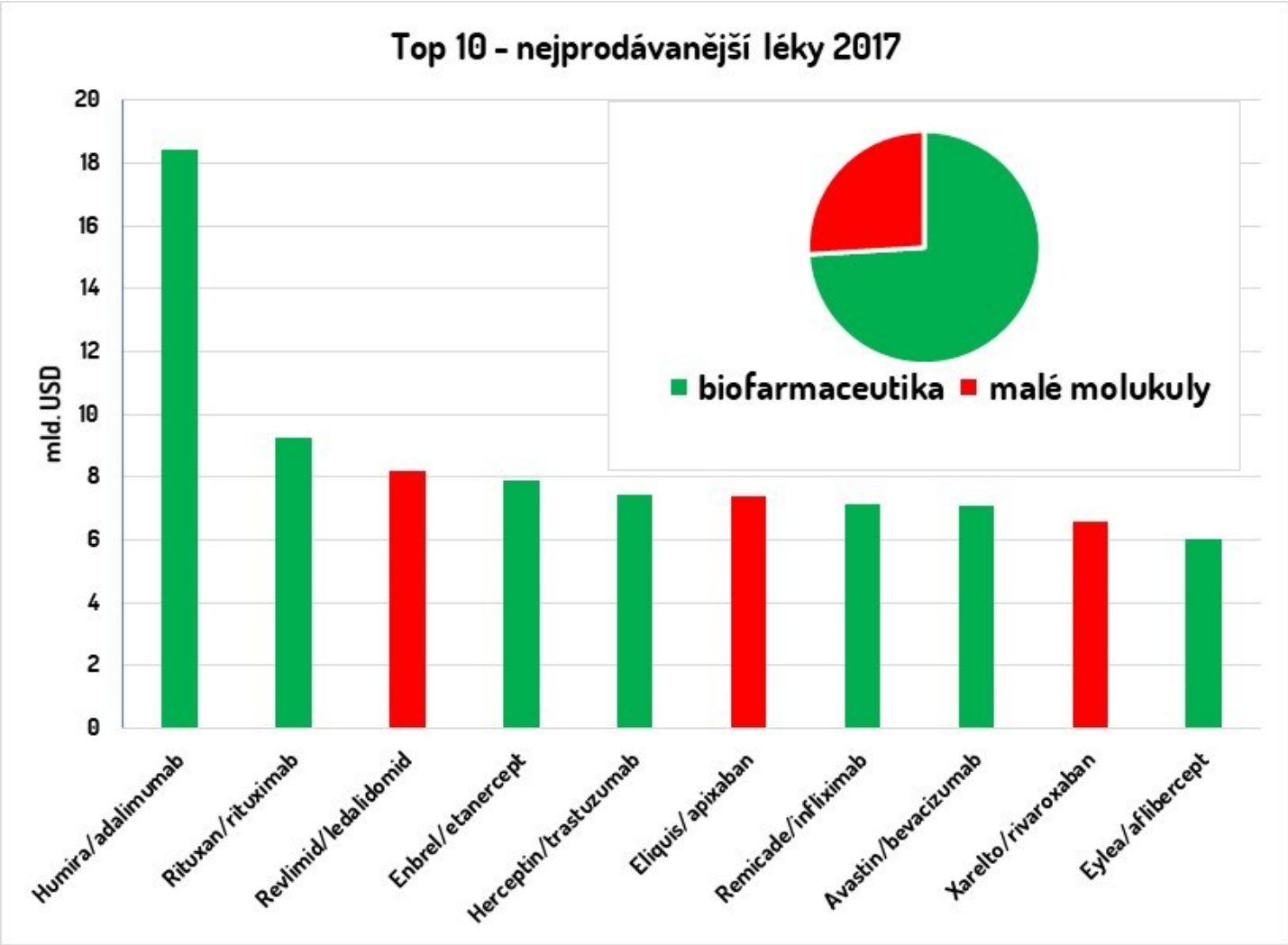




pragolab

ThermoFisher SCIENTIFIC

CO TO JE? PROČ?



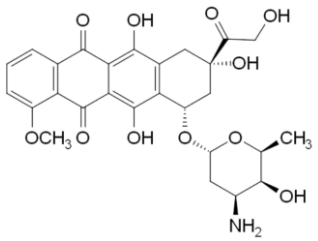
-UMAB

-XIMAB

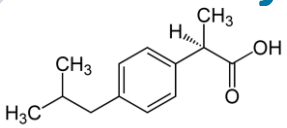
-ZUMAB

-ERCEPT

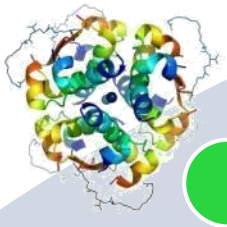
ANALYTICKÉ VÝZVY



Malé molekuly

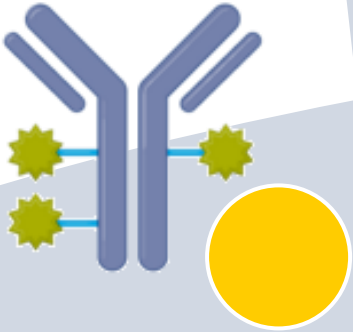


Chemoterapeutika



Malé proteiny

Protilátky mAb

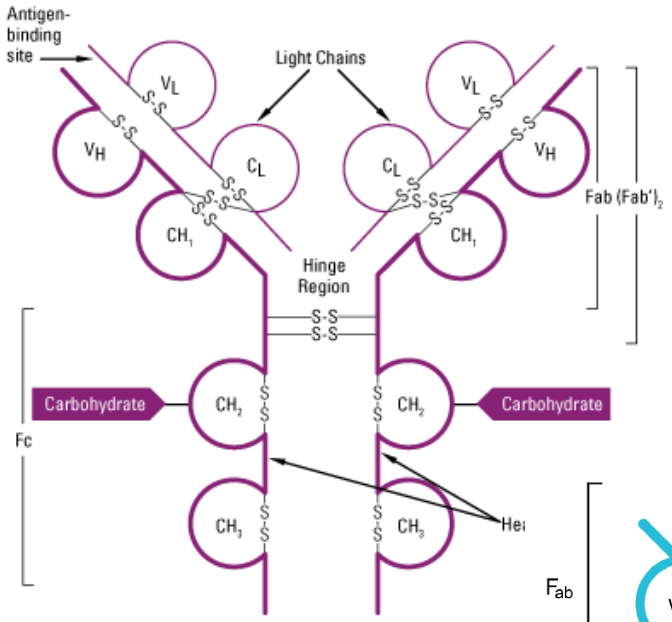


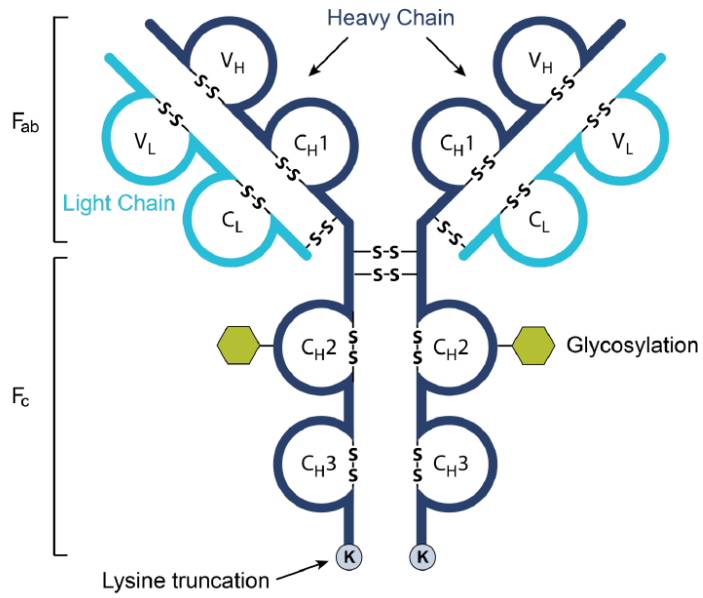
Antibody-Drug Conjugate

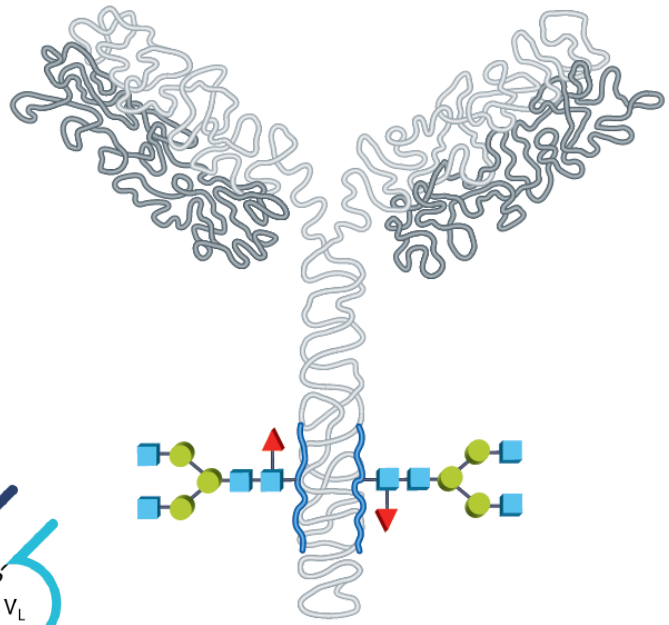
adalimumab

$C_{6428}H_{9912}N_{1694}O_{1987}S_{46}$

ANALYTICKÉ VÝZVY

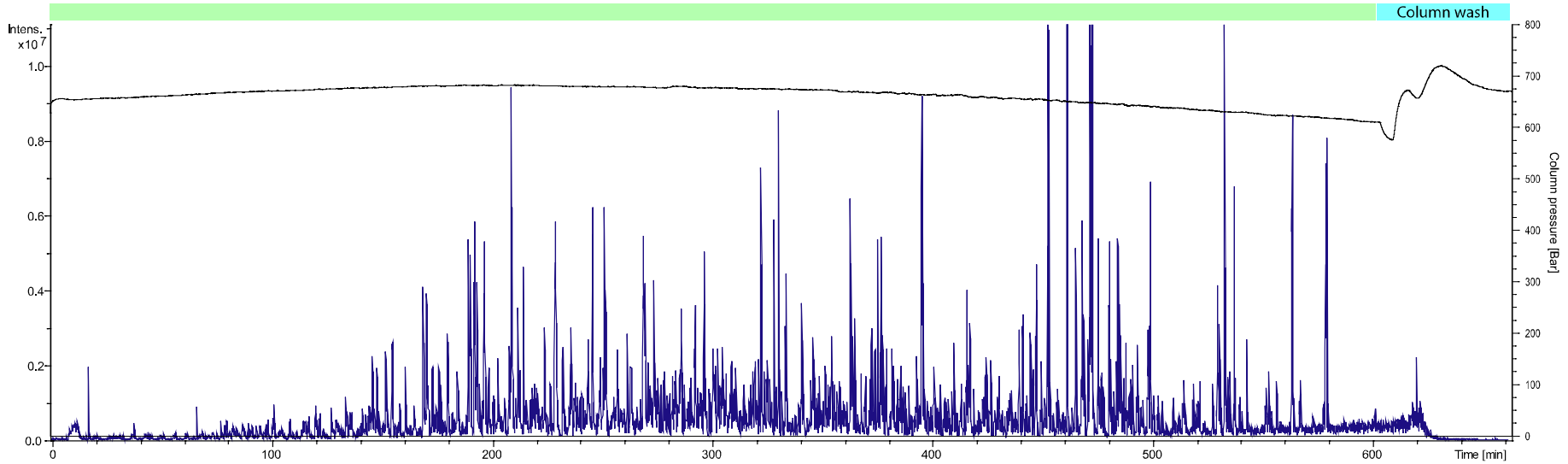






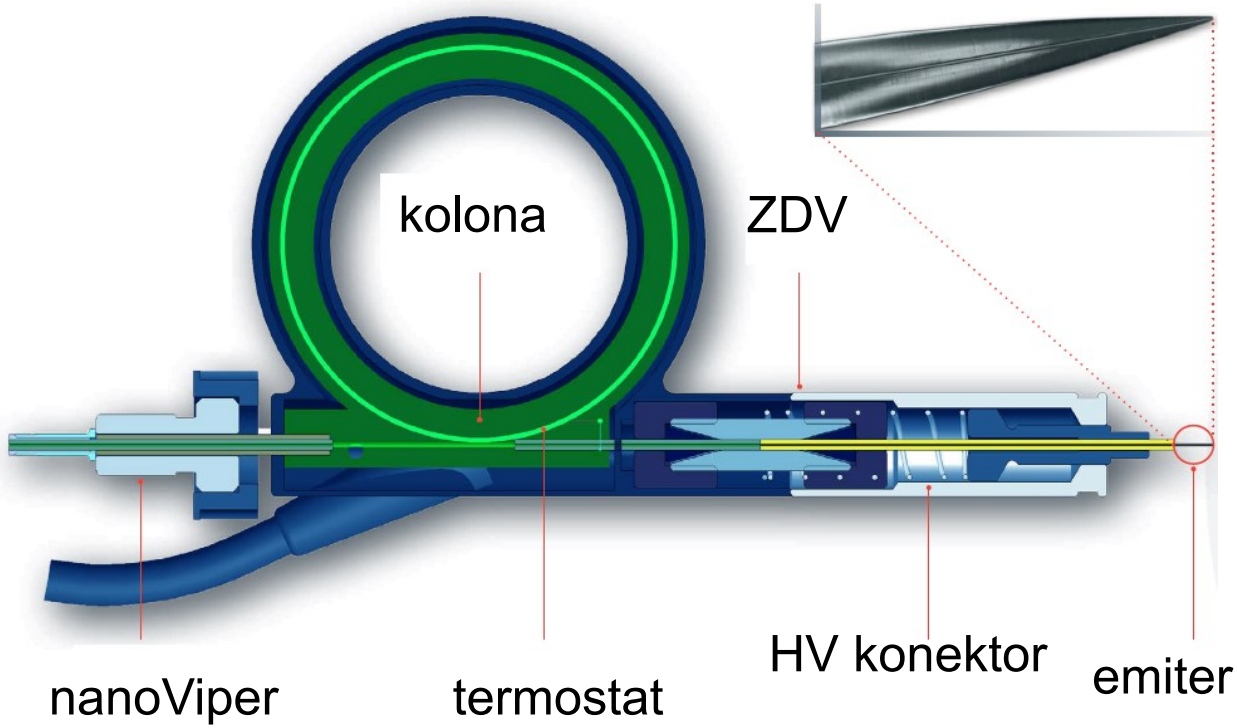
UHPLC analýza velkých molekul

- Acclaim PepMap RSLC C18, 2 µm
- 75 µm ID x 50 cm
- 650 – 700 bar @ 270 nL/min
- Gradient: 3 – 50% B, 600 min
- e. Coli digest



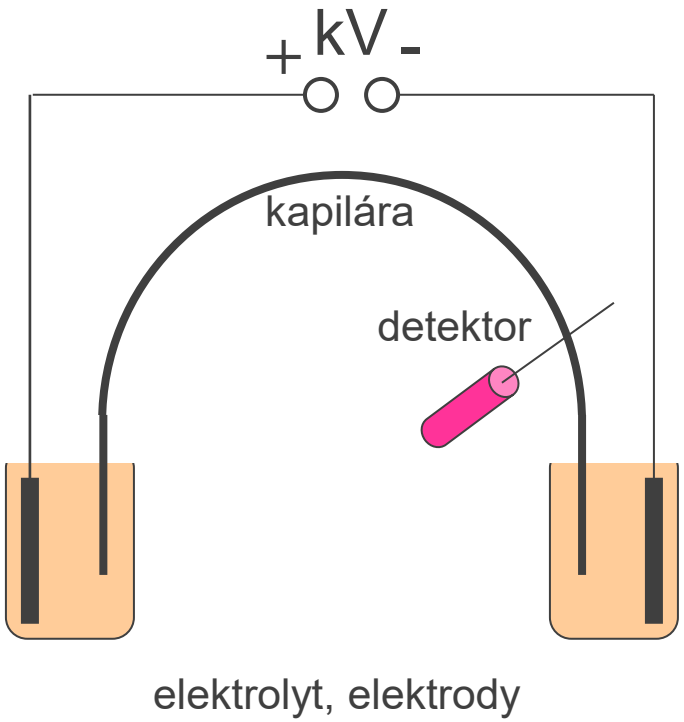
1 000 píků, 10 000 peptidů

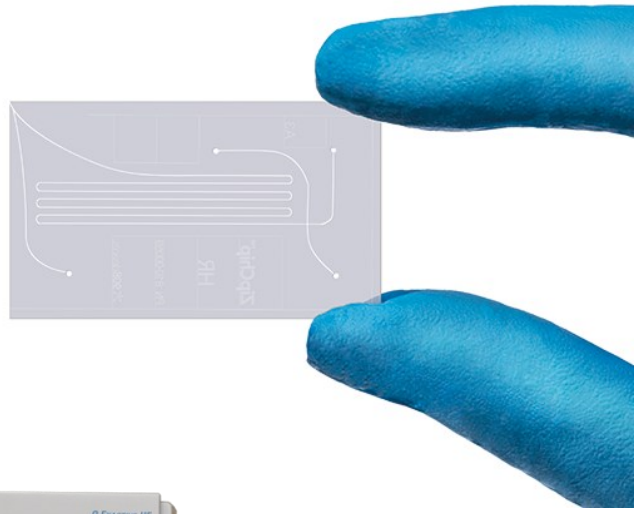
Integrovaná kolona v iontovém zdroji



EasySpray

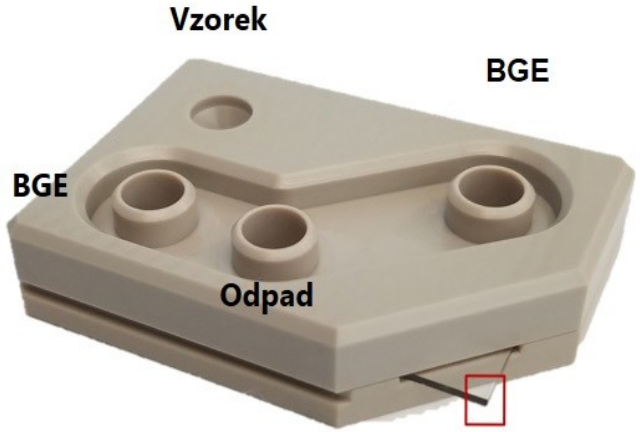
Integrovaná kap. elektroforéza v iontovém zdroji

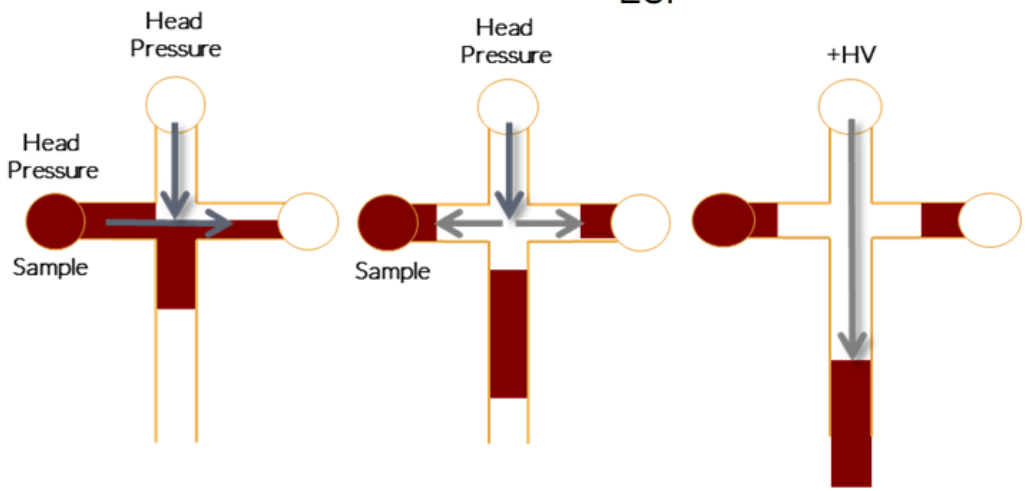


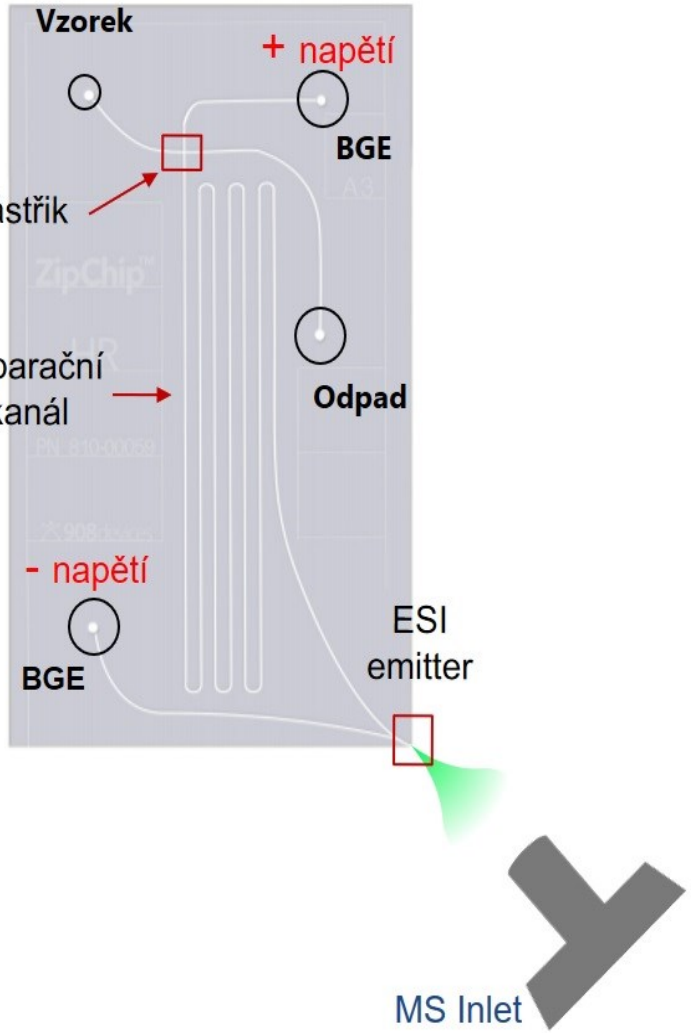


ZipChip

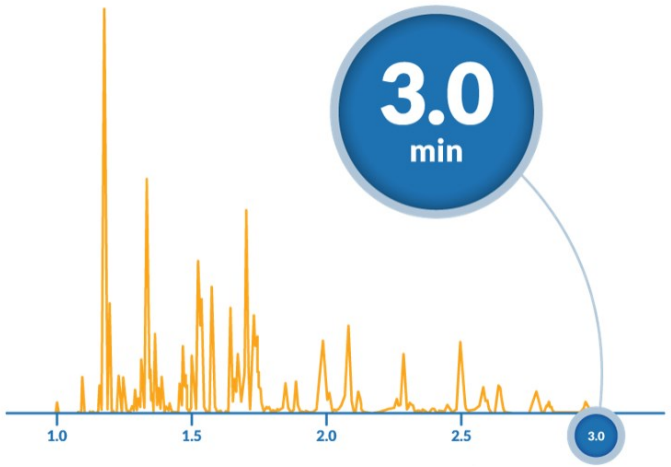
Integrovaná kap. elektroforéza v iontovém zdroji

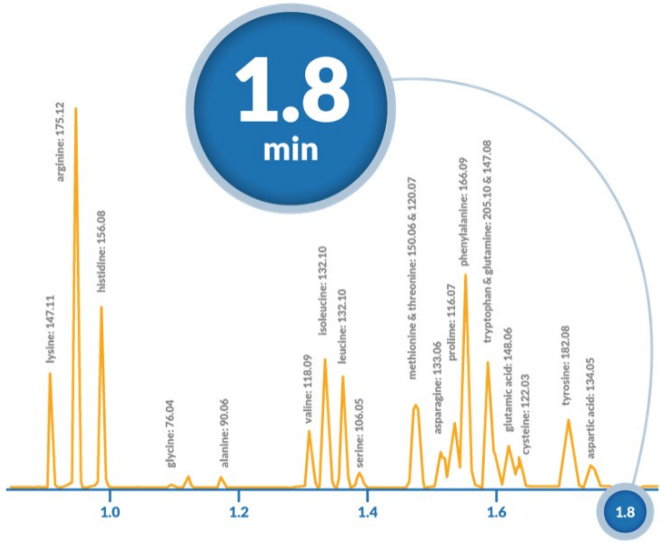


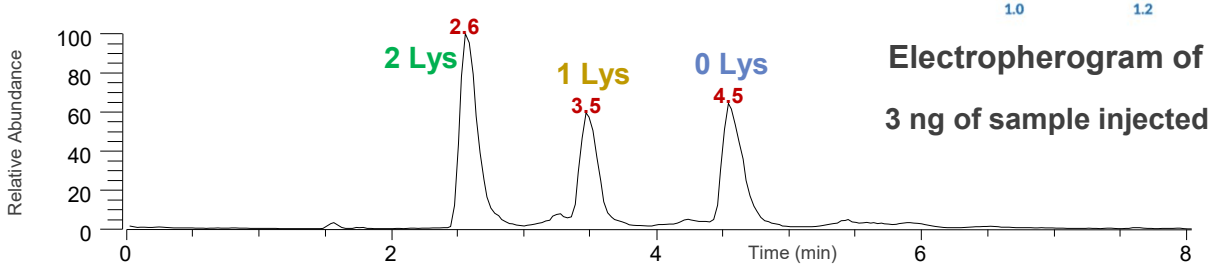




Integrovaná kap. elektroforéza v iontovém zdroji



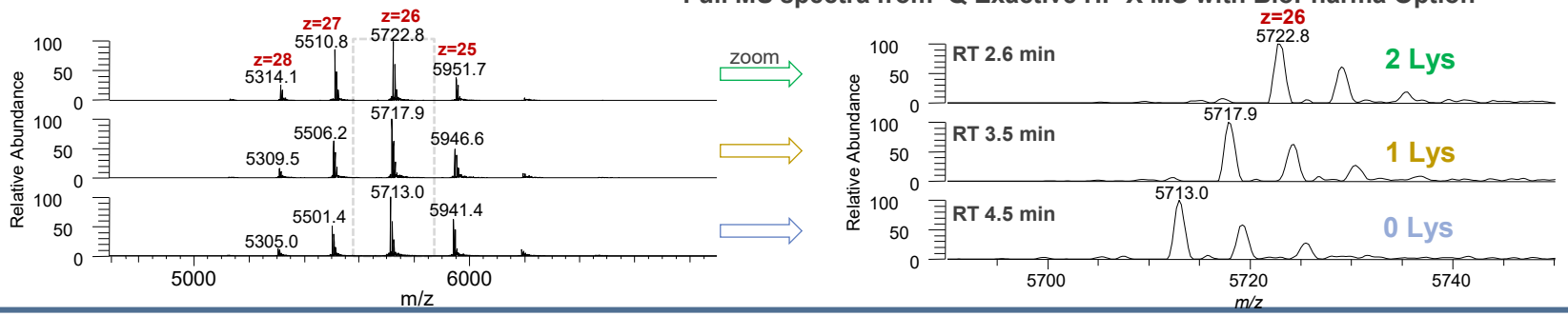




Electropherogram of intact infliximab:

3 ng of sample injected

Full MS spectra from Q Exactive HF-X MS with BioPharma Option



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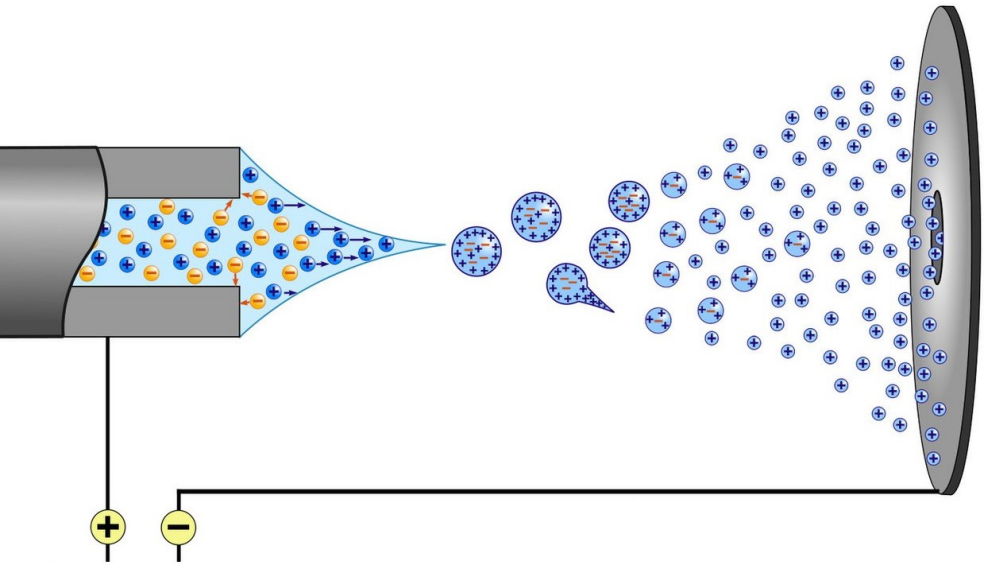
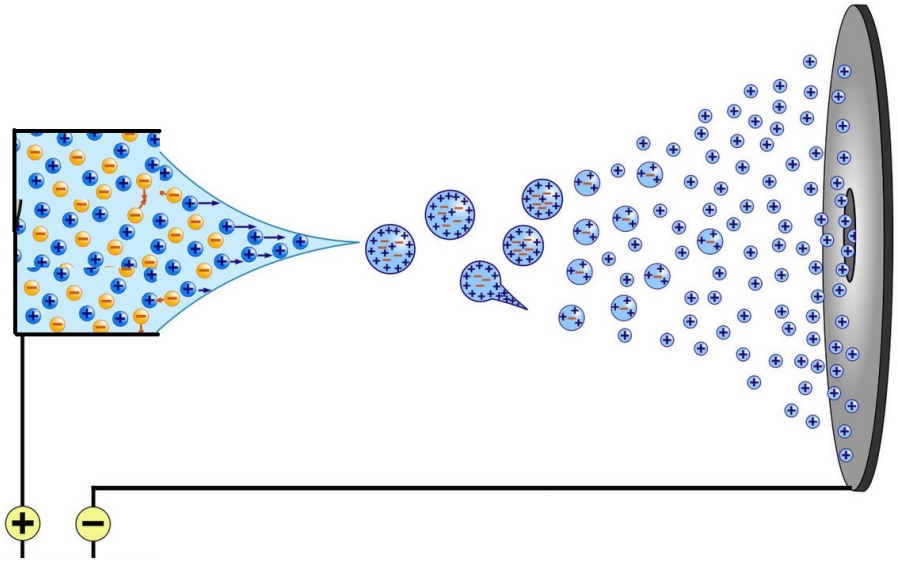
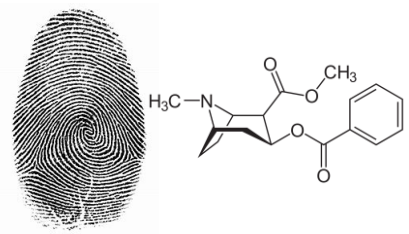
Integrovaný PaperSpray



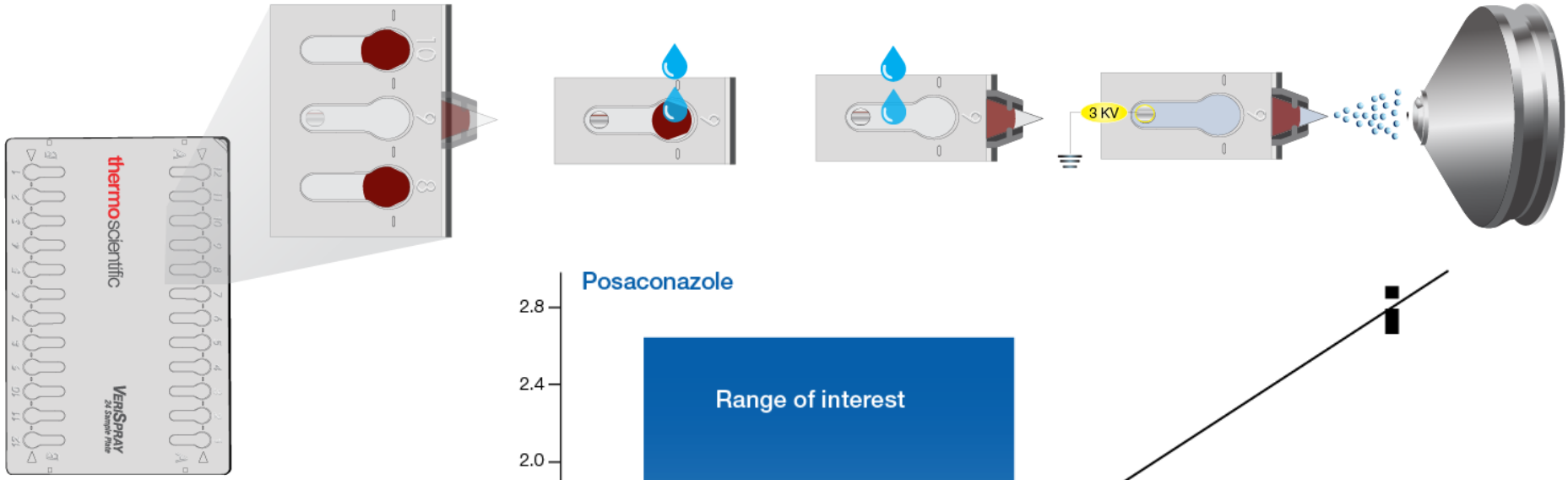
ElectroSpray



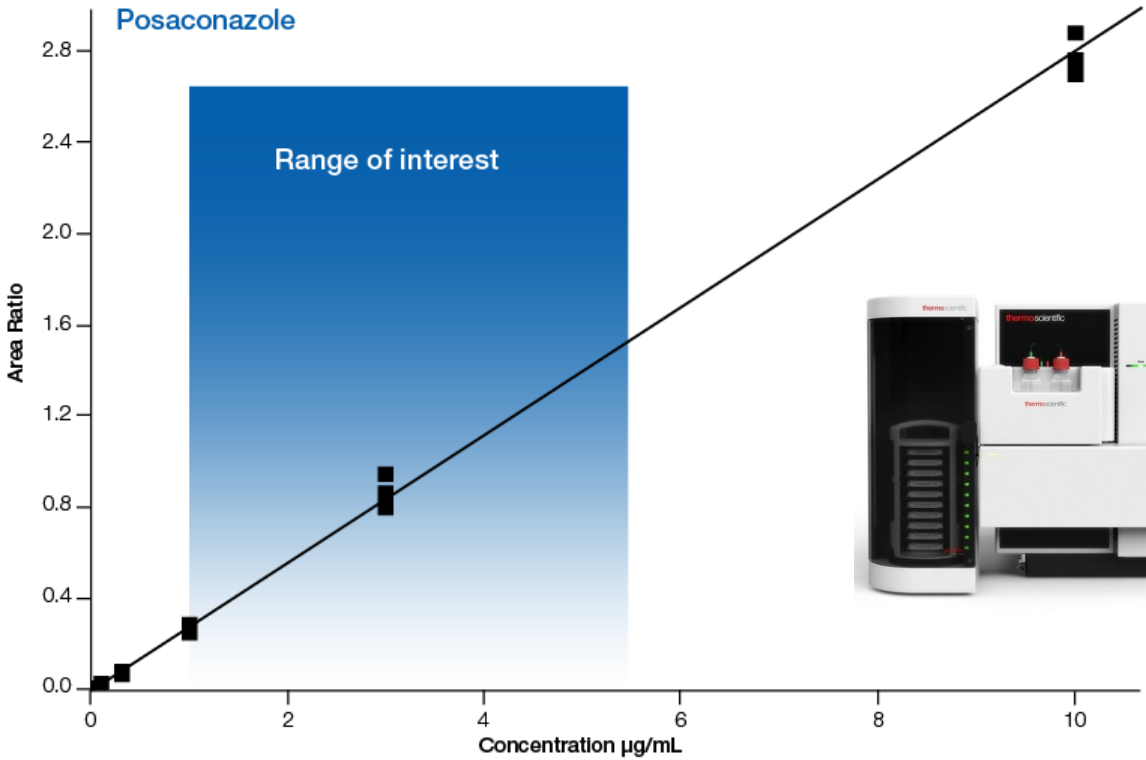
PaperSpray



Integrovaný PaperSpray



PaperSpray



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Extrahovatelné a louhovatelné látky (E&L)

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Extrahovatelné a louhovatelné látky (E&L)

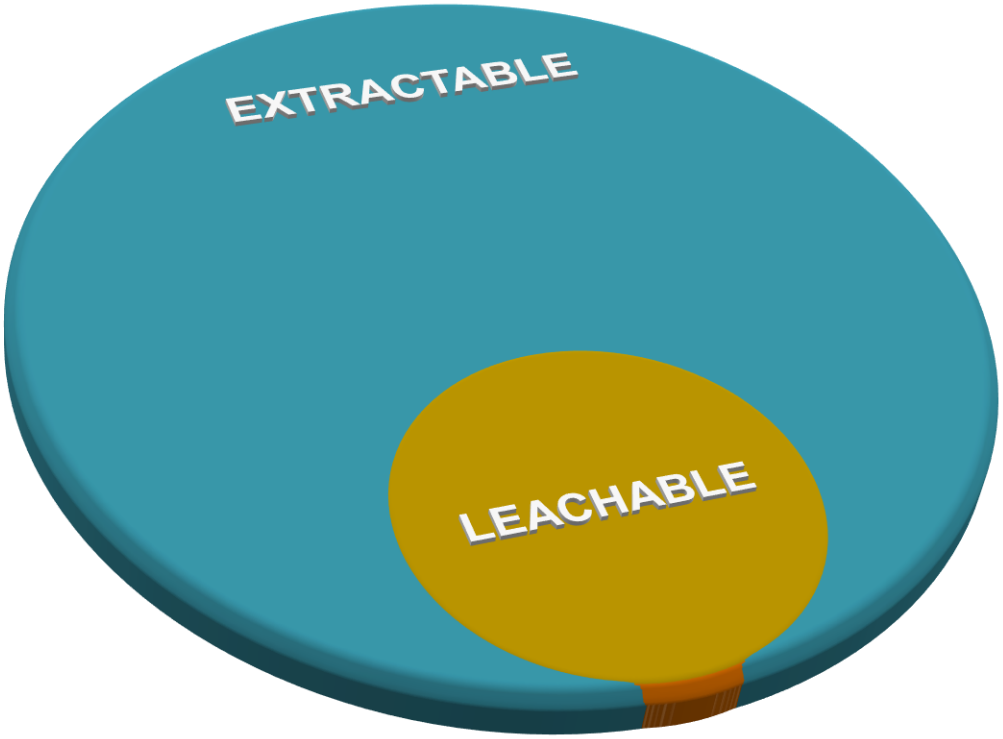
EXTRACTABLE

Chemické látky, které se **uvolňují** ze zařízení nebo obalu za **laboratorních podmínek extrakce**.

Proces nesmí degradovat ani deformovat materiál.

LEACHABLE

Chemické látky, které **migrují** z výrobního procesu, balení nebo transportu do lékové formy za **normálních podmínek užívání**.



L jsou většinou podmnožinou E

Extrahovatelné a louhovatelné látky (E&L)

- Etiketa
  - inkoust
  - solvent
  - lepidlo
  - lak
- Obal
  - změkčovač
  - lubricant
  - pigment
  - stabilizátor
  - antioxidant
  - monomery
  - retardant hoření

- Krabička
  - sterilizační přísada
  - konzervant
  - potisk

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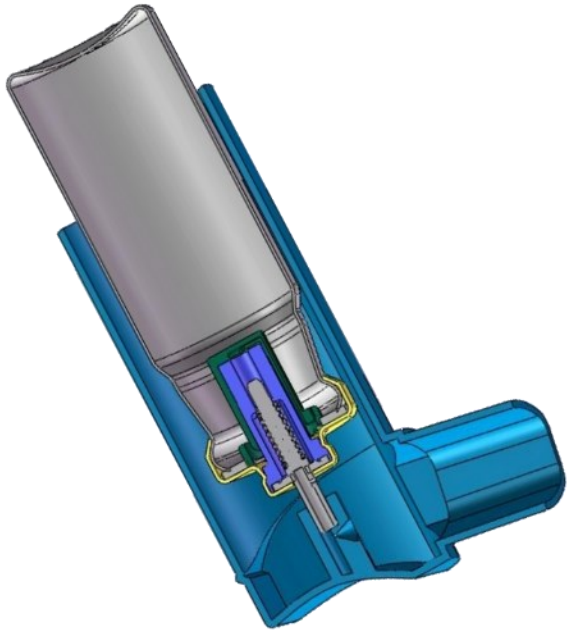
Extrahovatelné a louhovatelné látky (E&L)

EXTRACTABLE

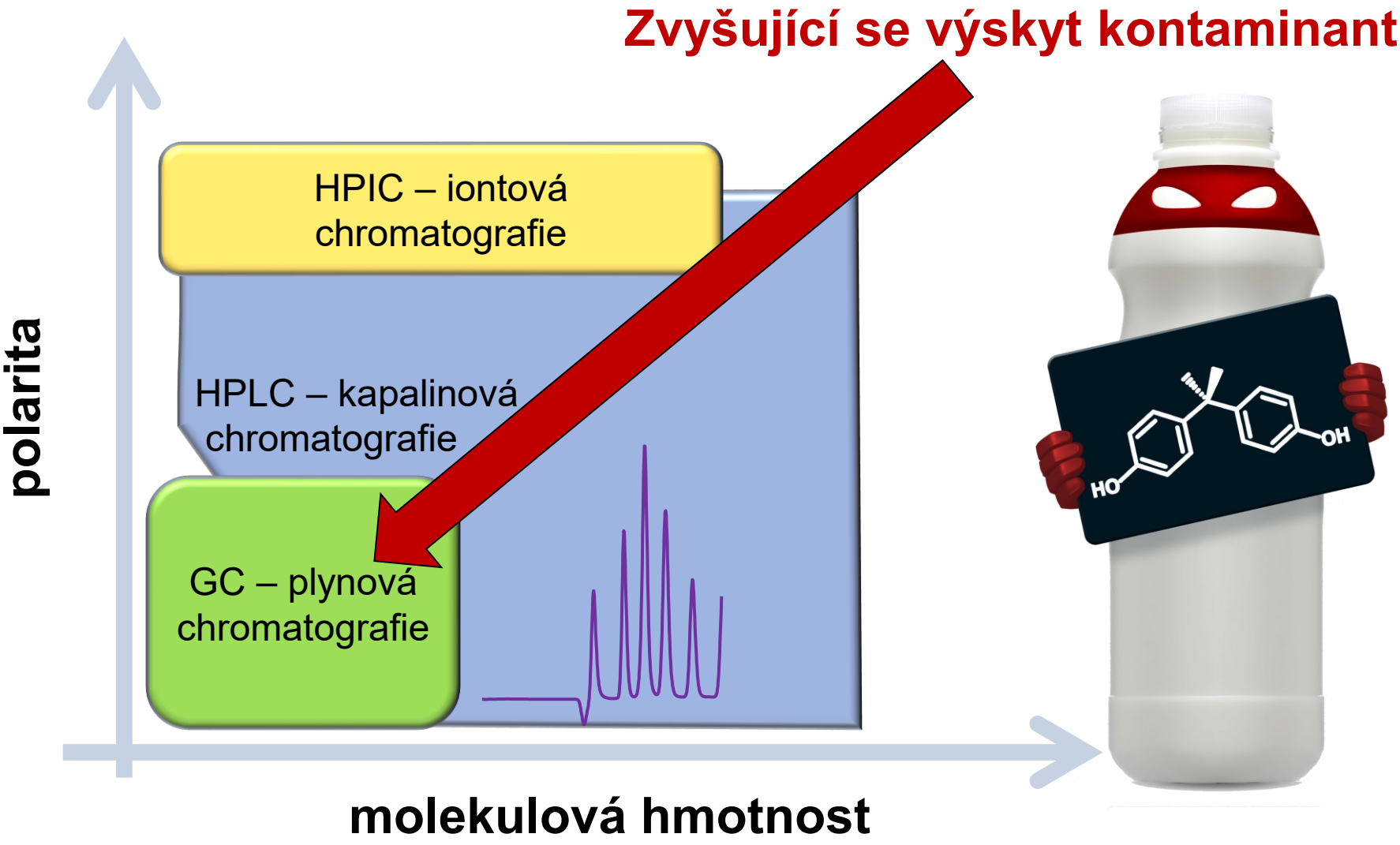


Testuje se materiál

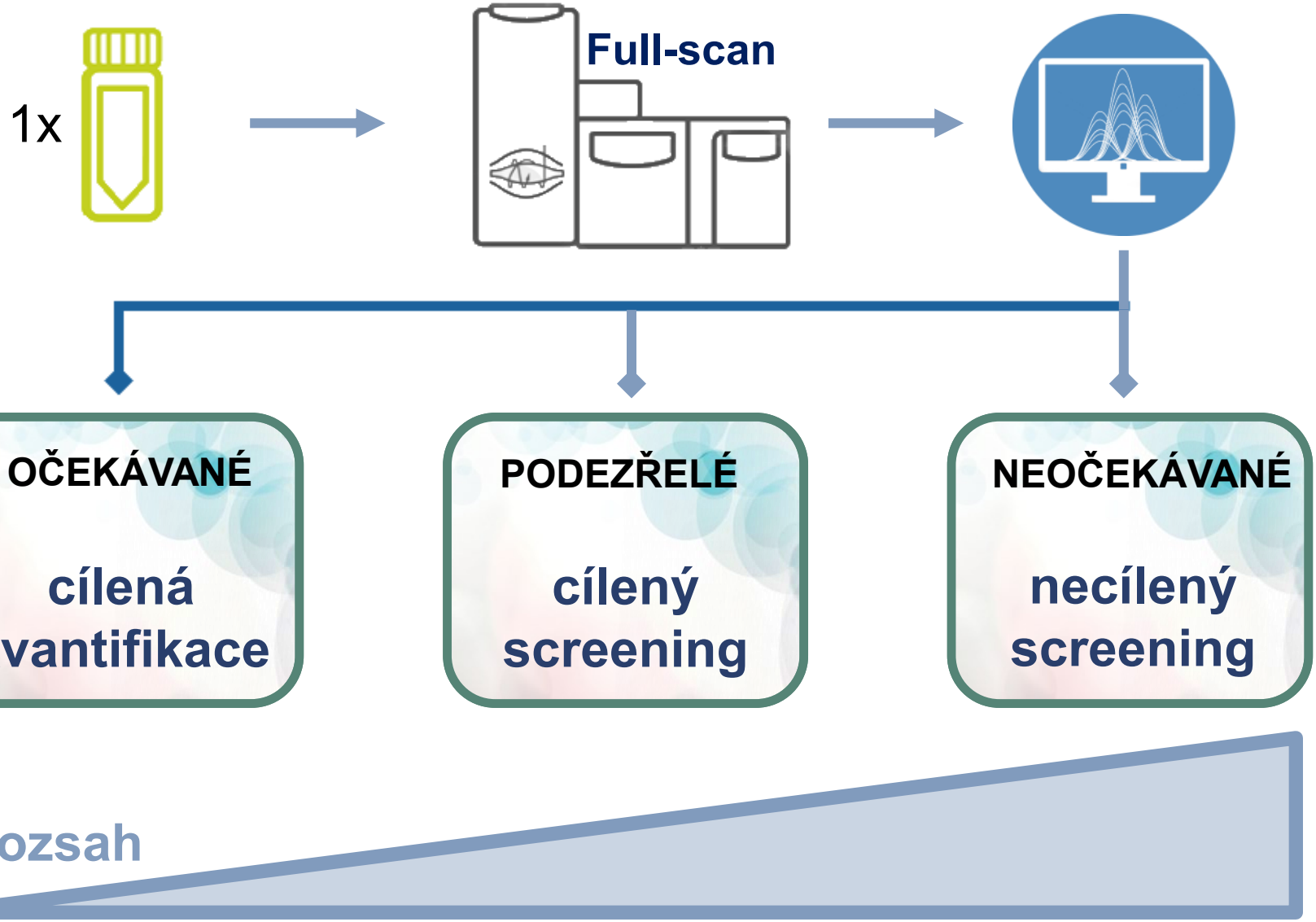
LEACHABLE

Testuje se produkt

Analytická separace



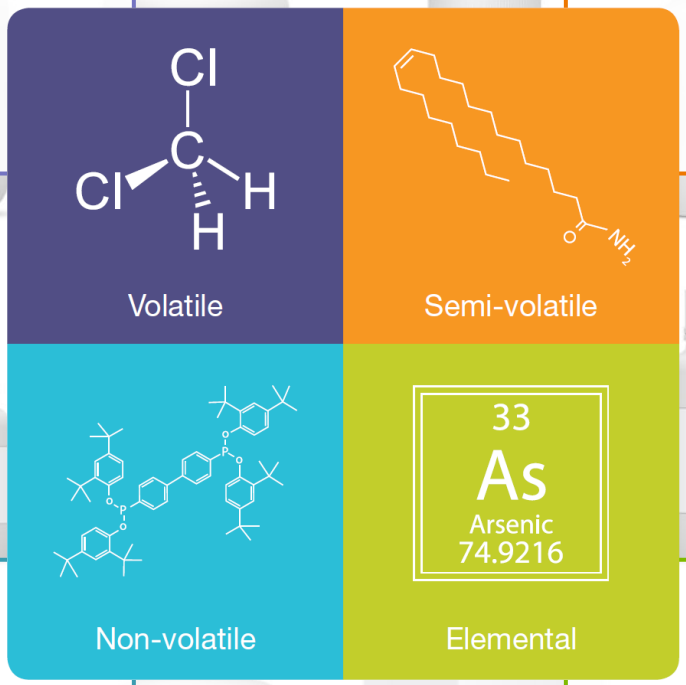
Cílená a necílená analýza



Analýza

- GC-MS
- GC-HRMS
- Headspace
- EI & CI
- Library

- GC-MS
- GC-MS/MS HRAM
- EI & CI
- Library



- ESI & APCI
- LC-UV or CAD
- LC-MS/MS HRAM
- IC-MS
- Library

- LC-ICP-MS
- IC-ICP-MS
- ICP-MS
- ICP-OES

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Komplexní řešení pro E&L

Preparation	Consumables	Volatiles	Semi-volatiles	Non-Volatiles	Elemental
					
Accelerated solvent extraction technology	MS certified vials, columns and ultra-pure solvents	Headspace sampling and compliant GC-MS	Advanced Orbitrap-based HRAM GC-MS/MS	Advanced Orbitrap-based HRAM LC-MS/MS	Robust, compliant ICP-MS

EXTRAKCE → **ANALÝZA A REPORTOVÁNÍ**

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Těkavé látky

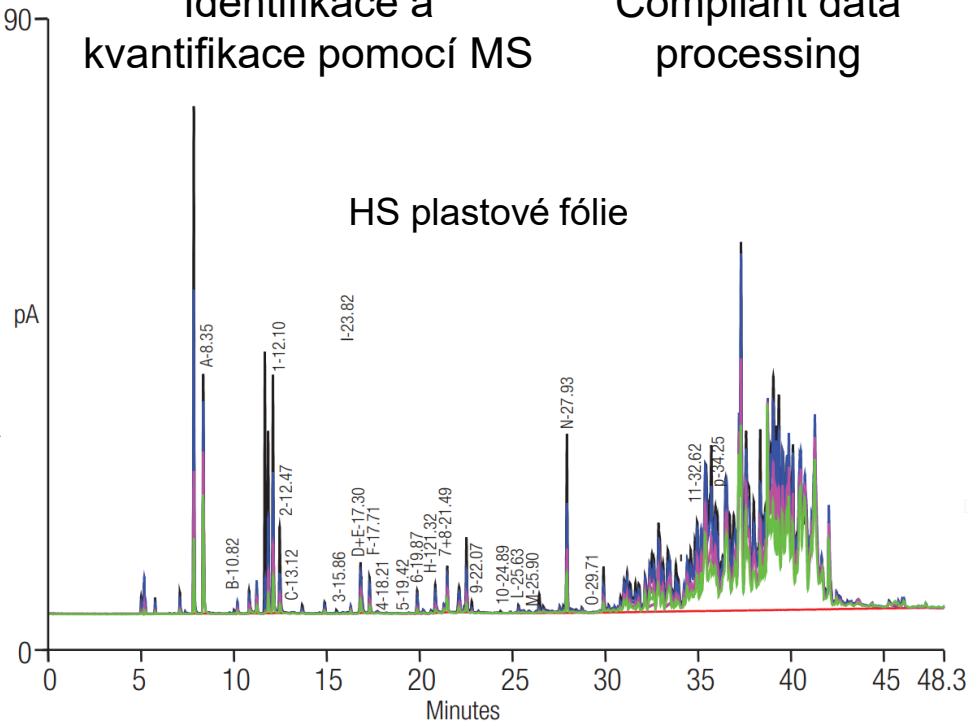
Vzorek + valve & loop headspace

Robustní separace

Identifikace a kvantifikace pomocí MS

Compliant data processing

- Analogické k **USP 467**
- Molekuly jsou obecně známé a **jednoduše kvantifikovatelné**



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Těkavé látky

Thermo Scientific™ TriPlus™ 300 headspace sampler

Thermo Scientific™ Trace 1310 GC

Thermo Scientific™ TraceGOLD TG-624SilMS GC Columns

Thermo Scientific™ ISQ™ Series GC-MS

Thermo Scientific™ Dionex™ Chromeleon™ CDS

Thermo Scientific™ AppsLab Library™

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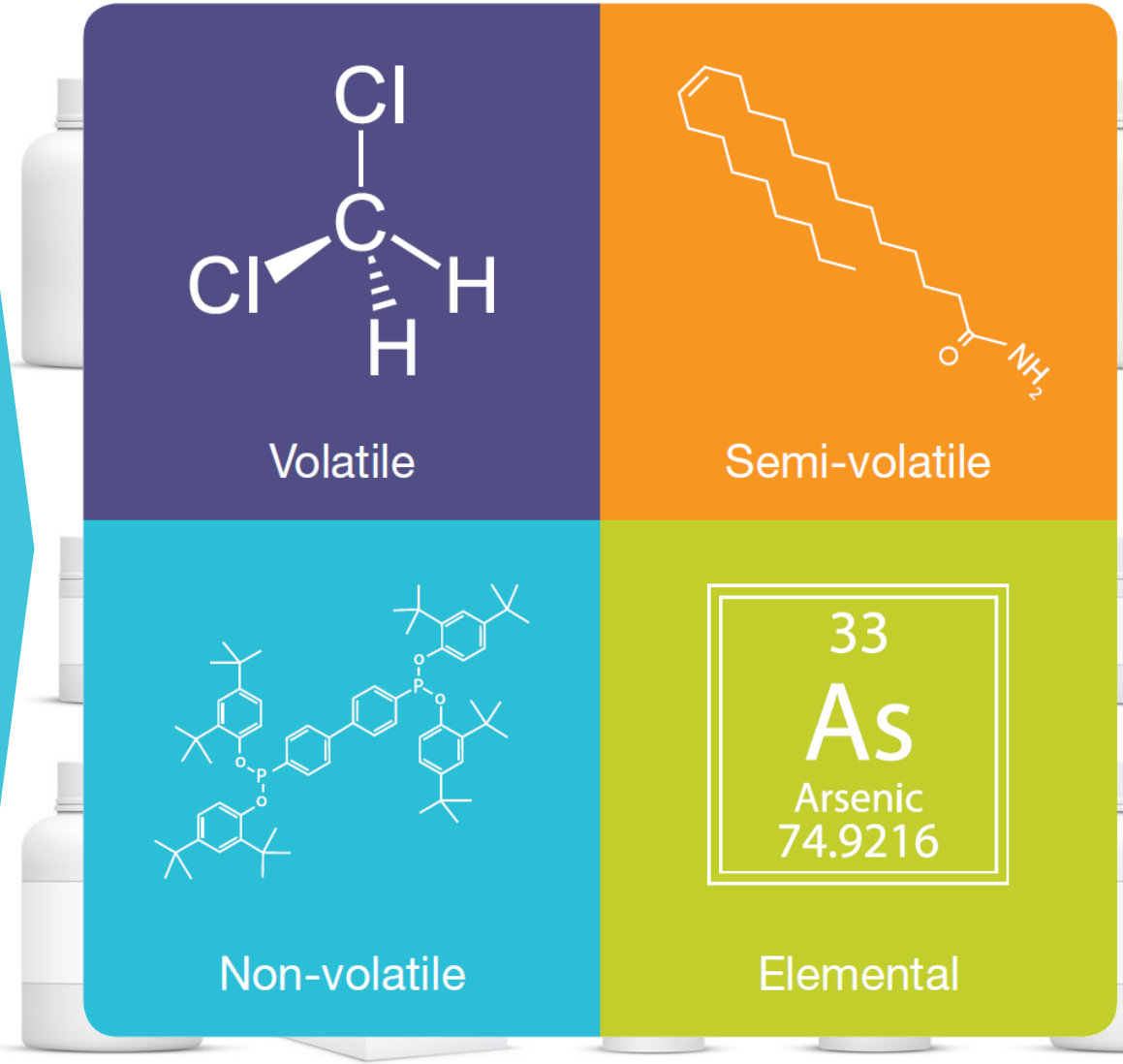
Netěkavé látky

Netěkavé



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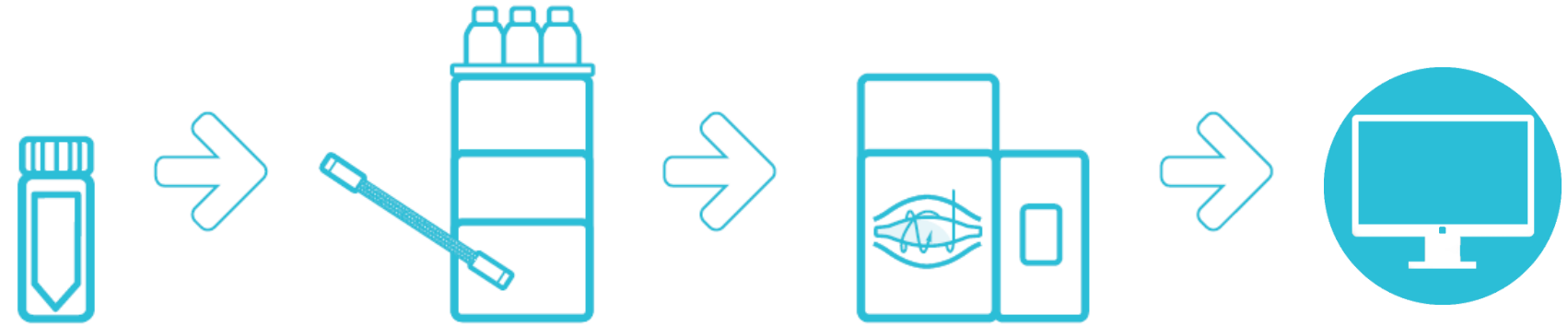
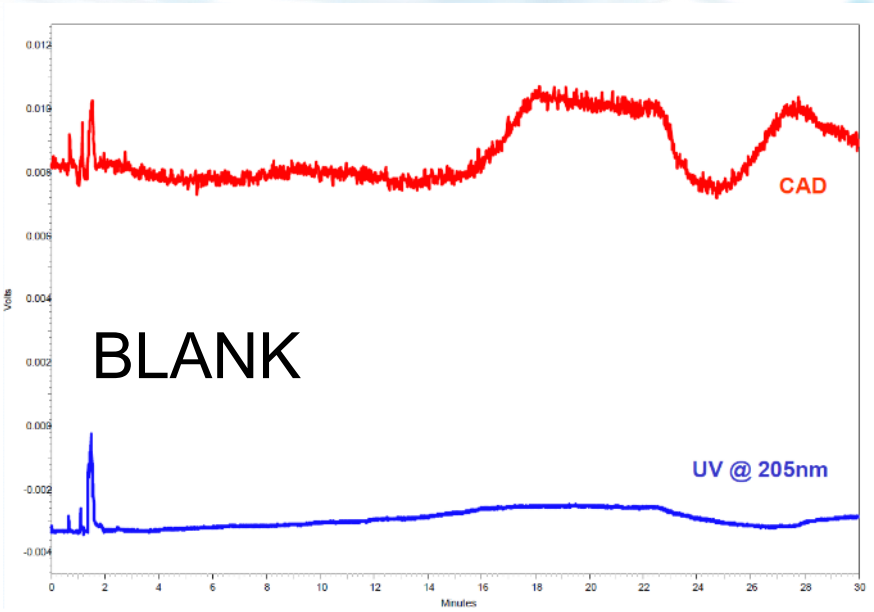
Netěkavé látky



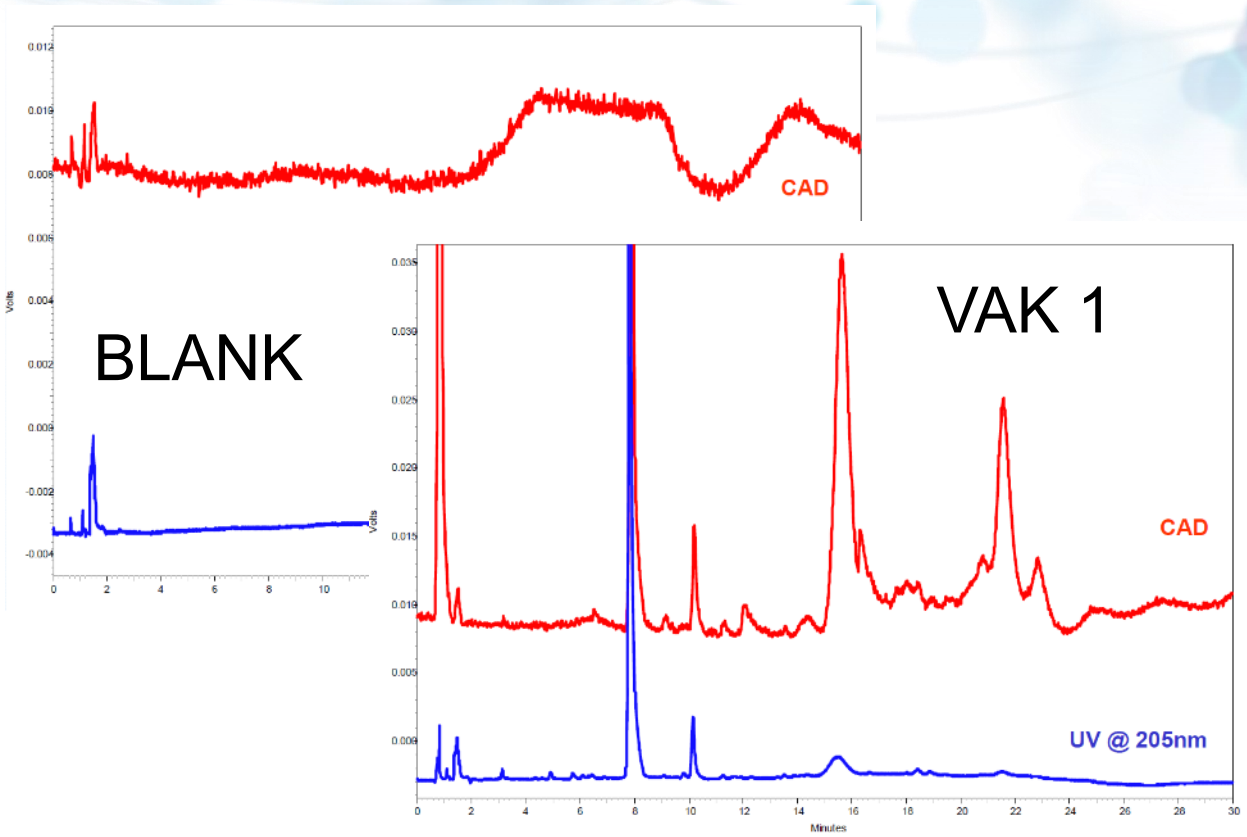
- Detekce v pozitivním i negativním módu
- **Elementární složení**
- Informace o struktuře (fragmentace)
- Zachytit vše – **kombinace s Corona CAD**

Netěkavé látky



Data from ESA Biosciences, Inc., Chelmsford, MA

Netěkavé látky



Data from ESA Biosciences, Inc., Chelmsford, MA

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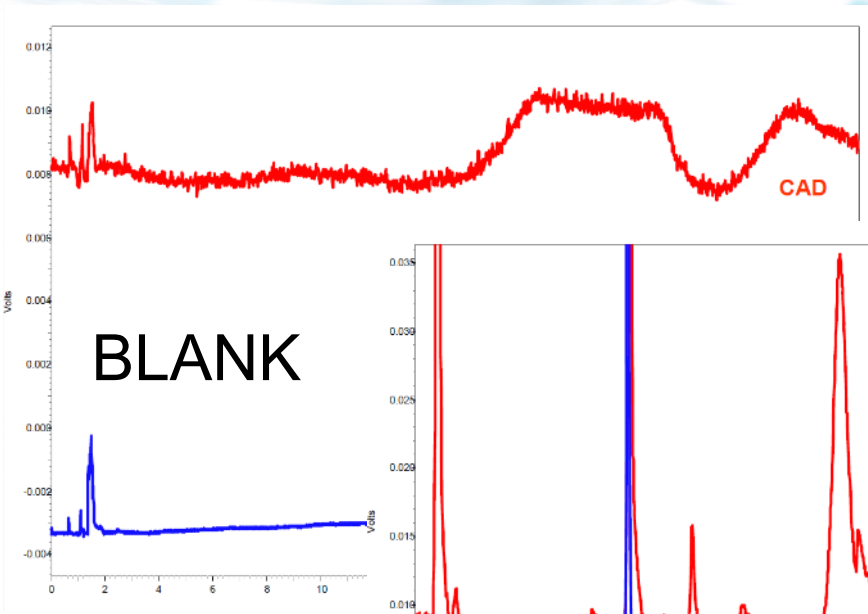
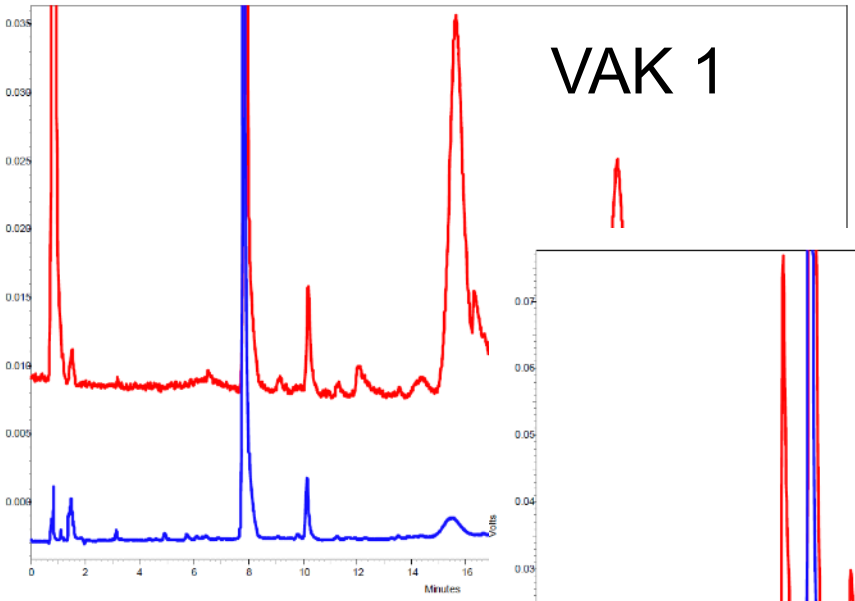
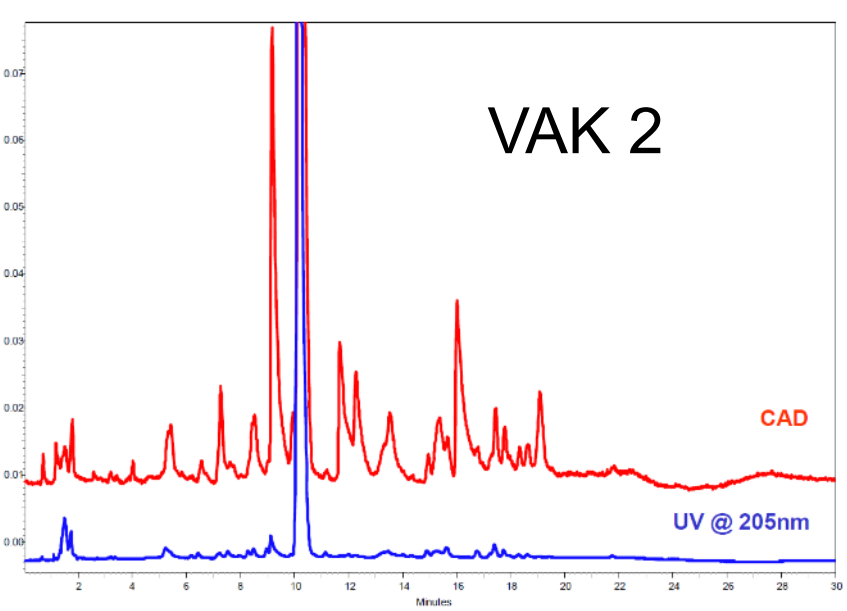
Netěkavé látky







120 nalezených látek

Data from ESA Biosciences, Inc., Chelmsford, MA

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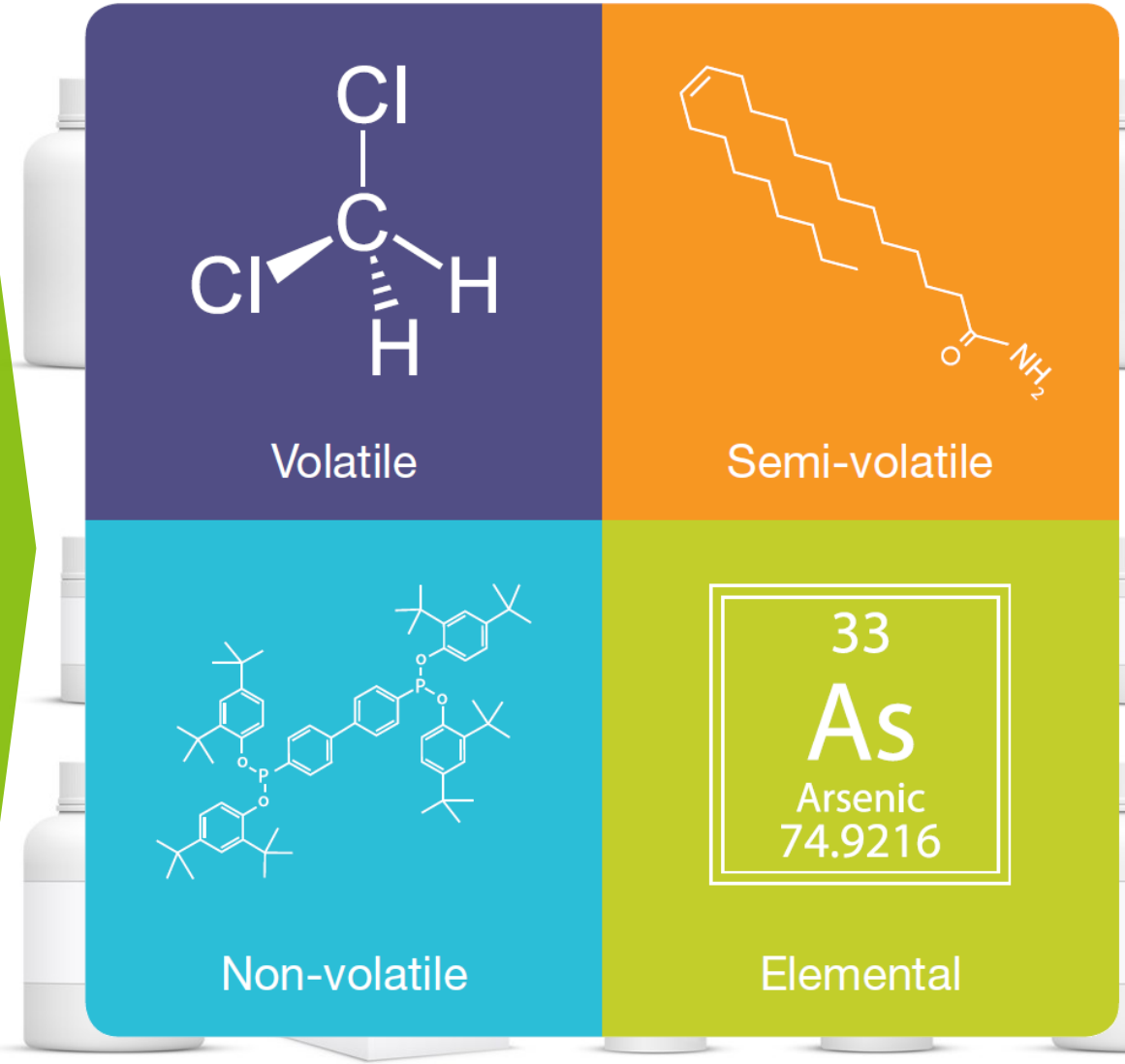
Prvková analýza

Kovy



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Prvková analýza

Extrakt | Automatická příprava vzorků | ICP-MS | Compliant data processing

- Analogické k **ICH Q3D a USP 232 & 233**
- Stopová analýza kovů, tolerance k org. matrici
- Thermo Scientific™ iCAP™ RQ ICP-MS

  - Stříbro (Ag) se uvolnilo ze 4 vaků
  - Olovo (Pb) se uvolnilo z 28 vaků

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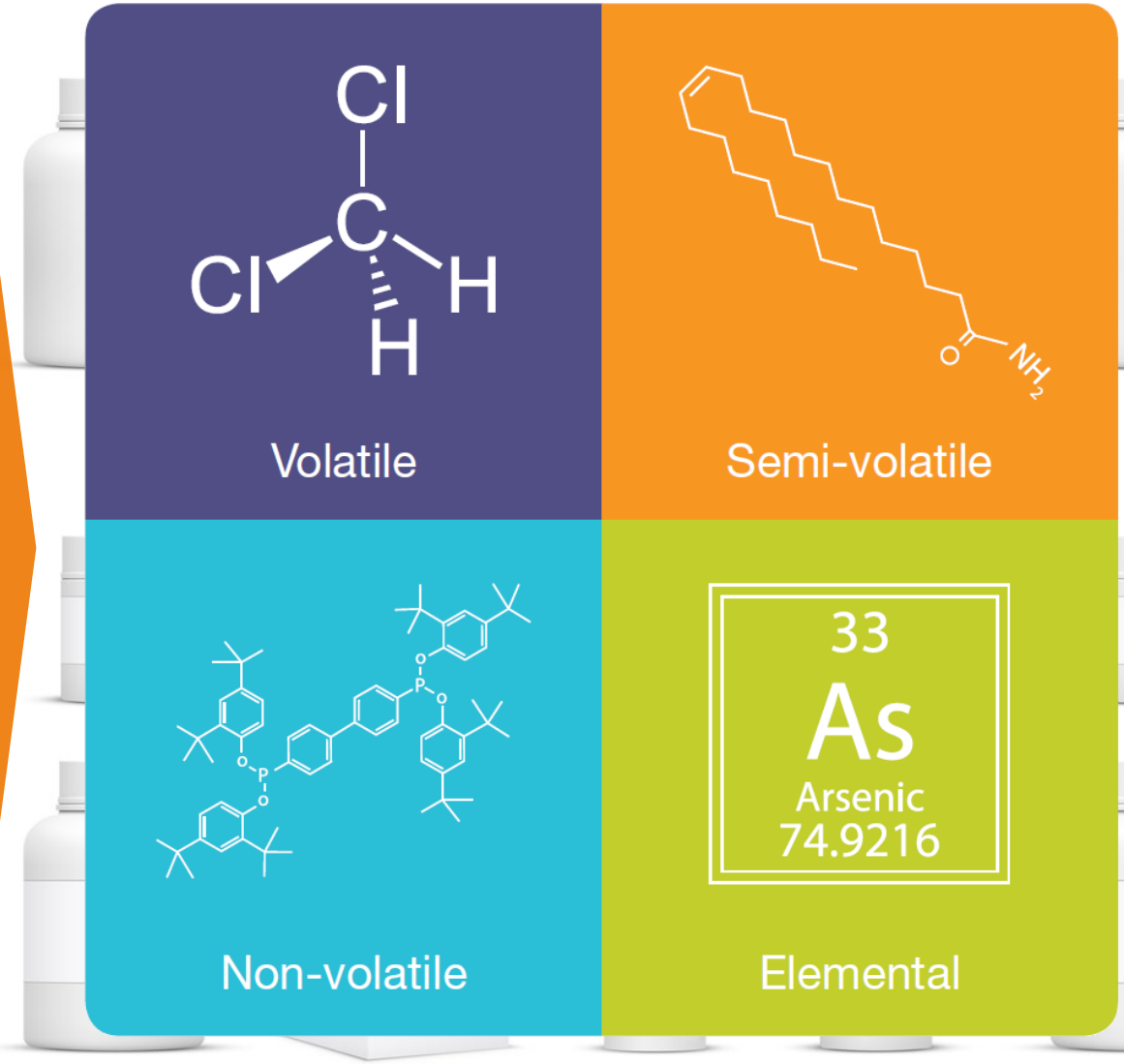
Odpařitelné, semi-volatilní

Semi-volatiles



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Odpařitelné, semi-volatilní

- EI/CI ionizace, full scan **HRMS 120k**
- Možnost MS/MS
- Excelentní SW podpora
- Thermo Scientific™ Q Exactive™ GC system

Identifikace

Q Exactive GC Hybrid Quadrupole-Orbitrap GC-MS/MS system

Trace 1310 GC system

TraceFinder software

TRACE 1310 GC Parameters	
Injection Volume (uL):	1
Liner	Single gooseneck
Inlet (° C):	280
Carrier Gas, (mL/min):	He, 1.3
Oven Temperature Program:	
Temperature 1 (°C):	40
Hold Time (min):	1
Temperature 2 (°C):	320
Rate (°C/min)	5.5
Hold Time (min):	12

Q Exactive GC MS Parameters	
Transfer line (°C):	280
Ionization type:	EI
Ion source(°C):	230
Electron energy (eV):	70
Acquisition mode:	Full scan
Mass range (Da):	50-700
Mass resolution (FWHM):	**120k**
Lockmass (m/z):	207.03235

Identifikace

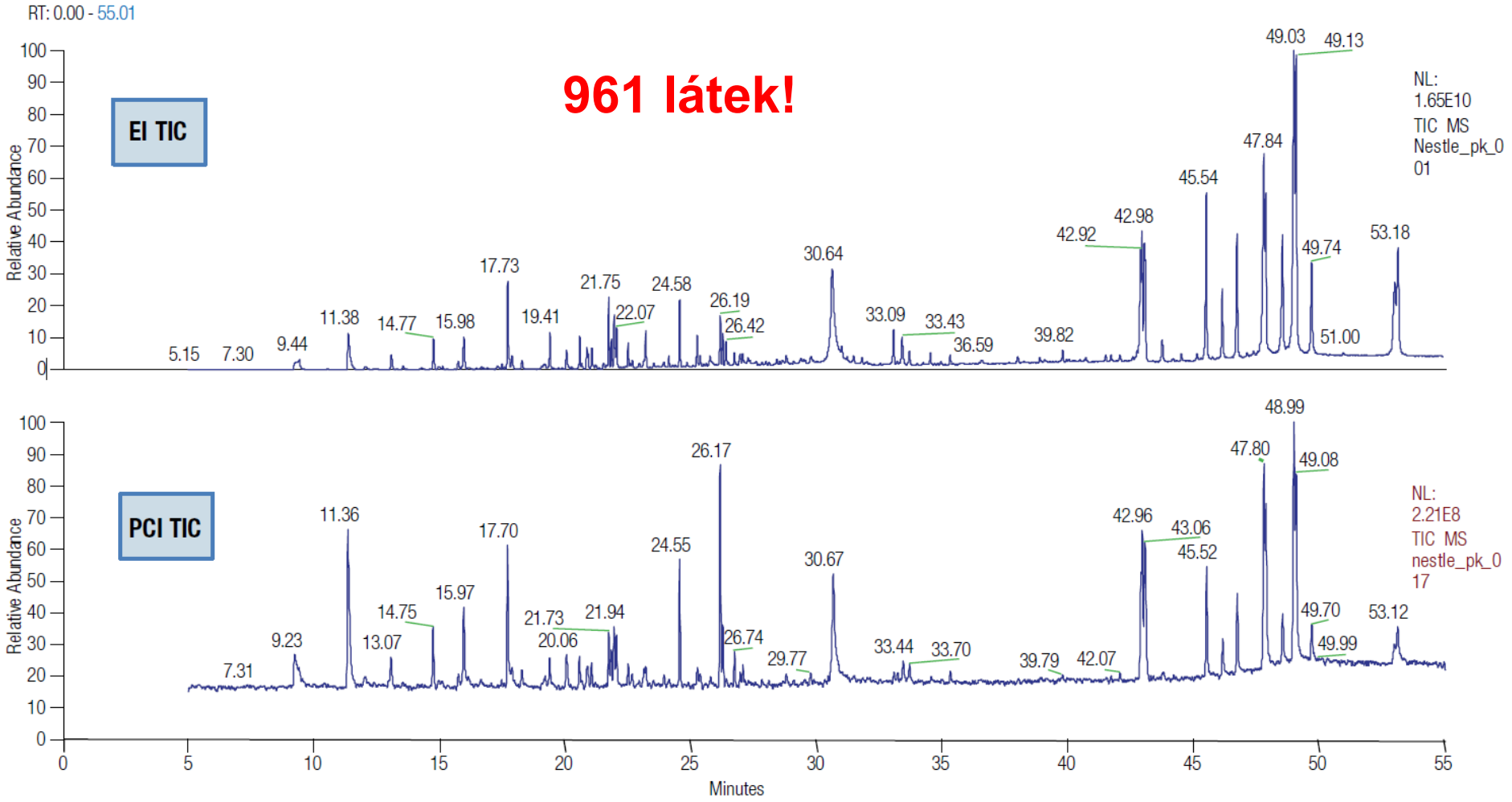
Vzorky těsnění

- **A** červené
- **B** hnědé
- **C** bílé
- **D** černé
- **Blank**

Plechovka

- **300 ml hexanu**
- **16 hod/lab. teplota**
- **Zakoncentrování na 1 ml**

Identifikace



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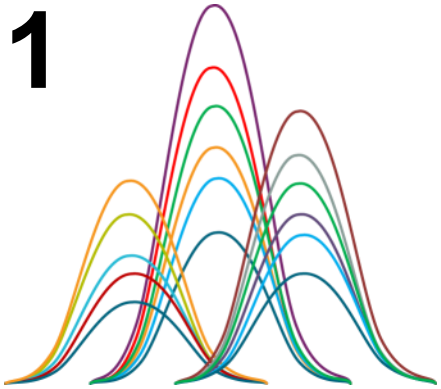
Identifikace

Detekce/dekonvoluce

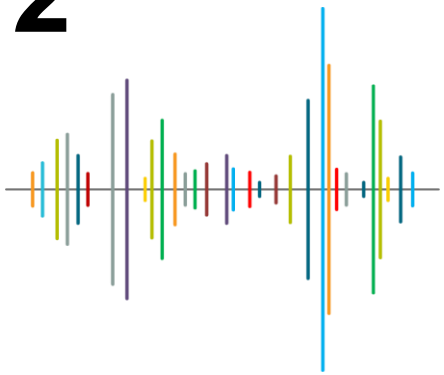
1



- detekcí píků
- HR dekonvoluce
- „čištění“ spektra

Generování kandidátů

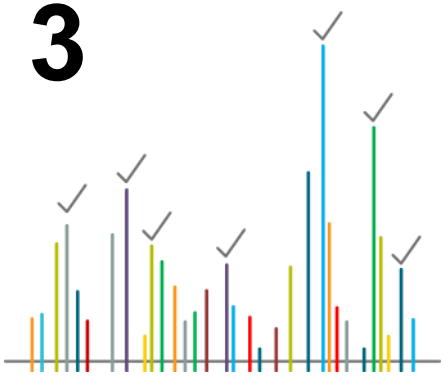
2



- hledání v knihovnách
- generování kandidátů

Filtrování, identifikace

3



- HR filtrování kandidátů
- hypotéza, identifikace

preferován (semi)automatizovaný proces

Identifikace

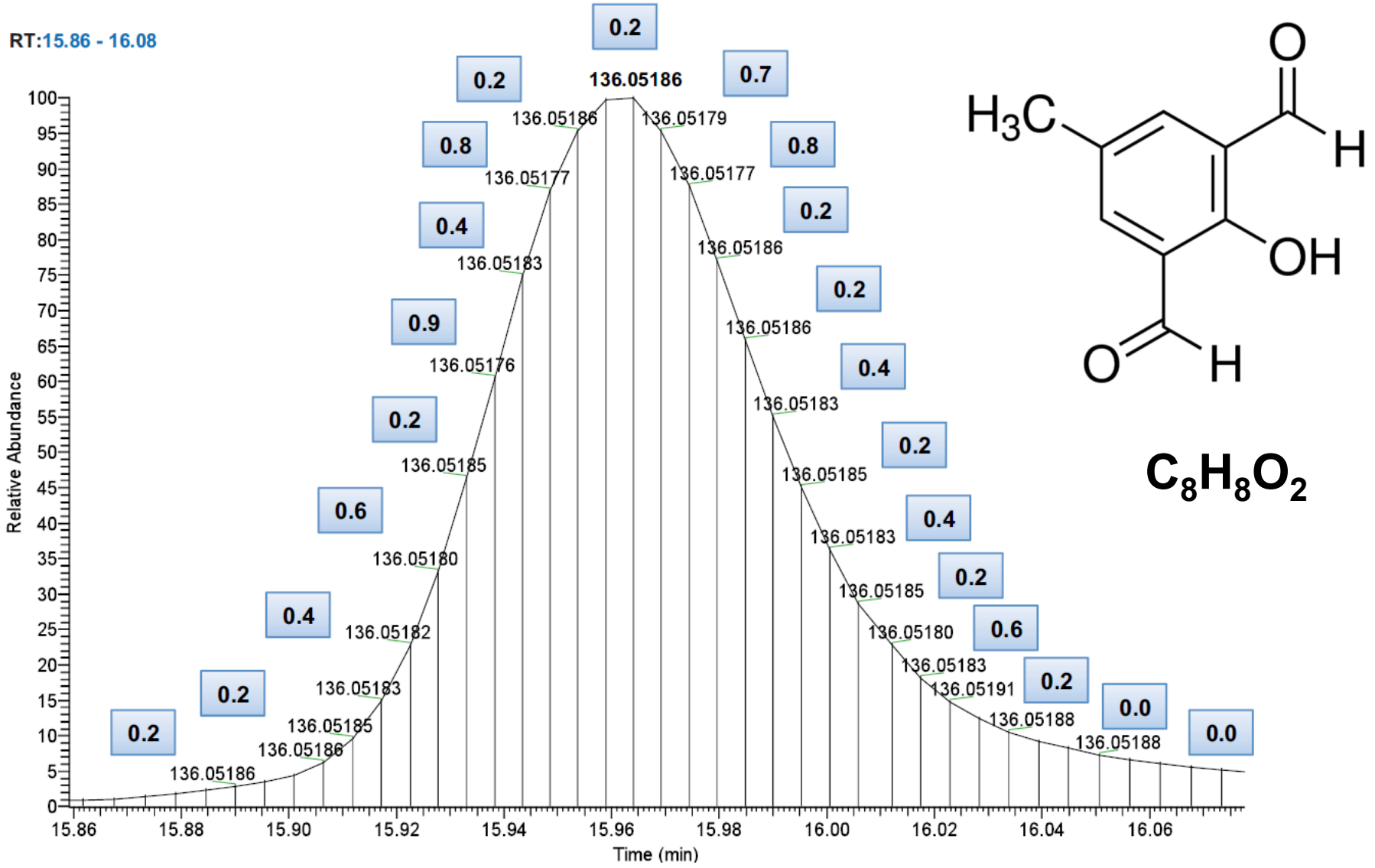
Kombinace SI (search index) a HRF (high resolution filtering) = hodnota skóre (%)

Pea entification

Score	Matched Compound	Formula	CAS	SI	HRF Score	M+ m/z	M+	M+ Lib	% Elements
94.4	**1,4-Dihydrophenacetic acid,...**	**C18H30O2**		**728**	**99.4959**	**278.22403**	**Yes**	**Yes**	**100**
70.4	1,5-Dioxaspiro[5.6]dodeca-7,...	C18H32O2Si2		524	99.8259	336.19353	No	Yes	100
57.7	Benzoic acid, 3,5-bis(1,1-dim...	C17H26O3	1620-64-0	706	58.9058	278.18764	No	Yes	100
56.8	3,5-di-tert-Butyl-4-hydroxyph...	C17H26O3	20170-32-5	659	58.9058	278.18764	No	Yes	100
55.4	Benzenemethanol, 3,5-bis(1,1...	C17H26O3	14387-17-8	591	58.9058	278.18764	No	Yes	100
51.3	Monoallyl phthalate, TBDMS ...	C17H24O4Si		517	52.4488	320.14383	No	No	100
44.5	2,6-Bis(tert-butyl)phenol, TMS...	C17H30OSi	10416-73-6	514	35.6312	278.20604	No	Yes	100
42.4	12-Cyclohex-3-enyl-3-methyl...	C23H24N2O		533	29.2285	344.18831	No	Yes	100
41.6	6-Oxo-5-phenyl-2,3,5,6-tetrah...	C16H13N3O	87365-22-8	525	27.7606	263.10531	No	Yes	100

$$\text{HRF skóre} = \frac{\sum (m/z * \text{Intenzita})_{\text{vysvětlené}}}{\sum (m/z * \text{Intenzita})_{\text{nalezené}}} \times 100\%$$

Identifikace



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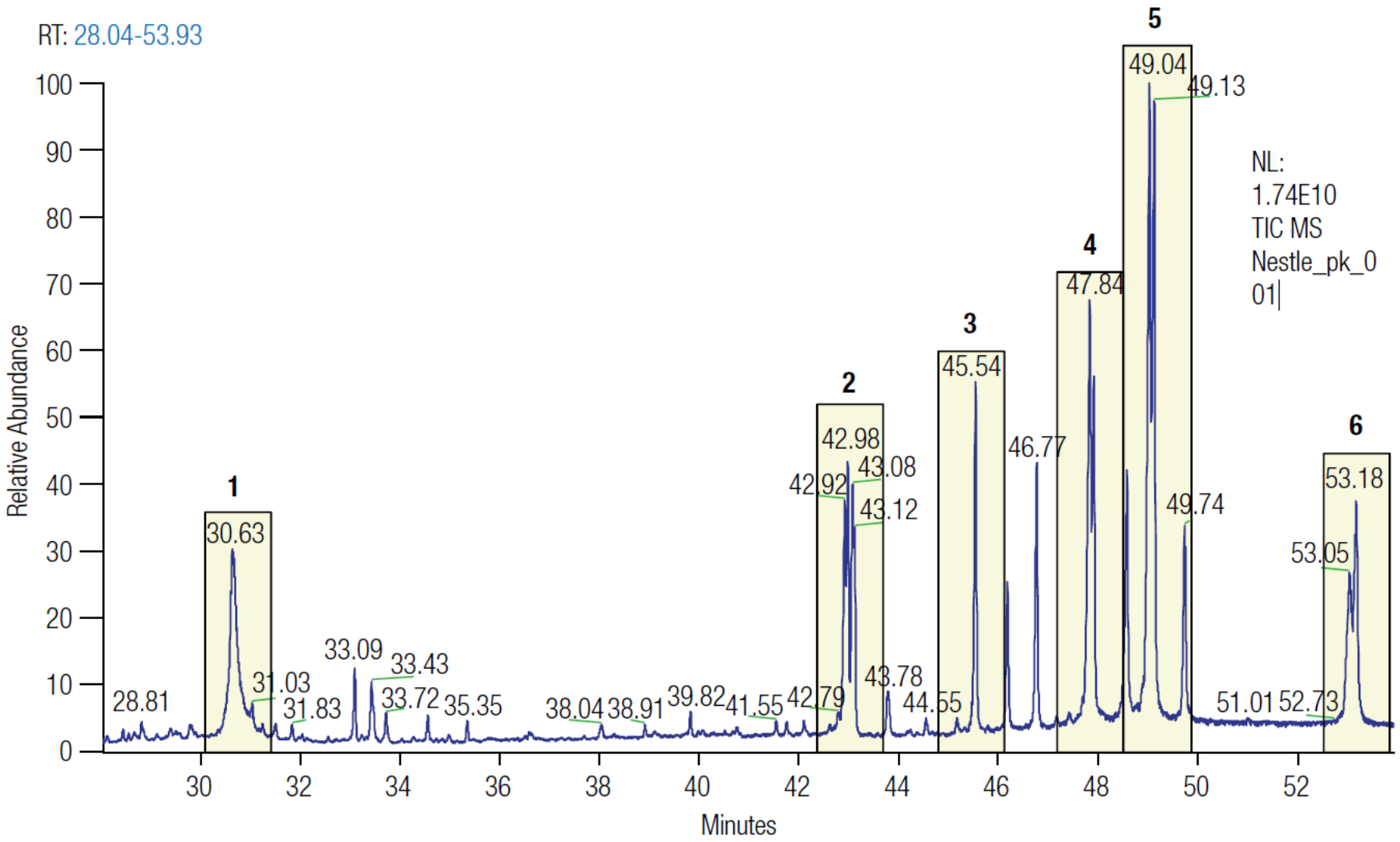

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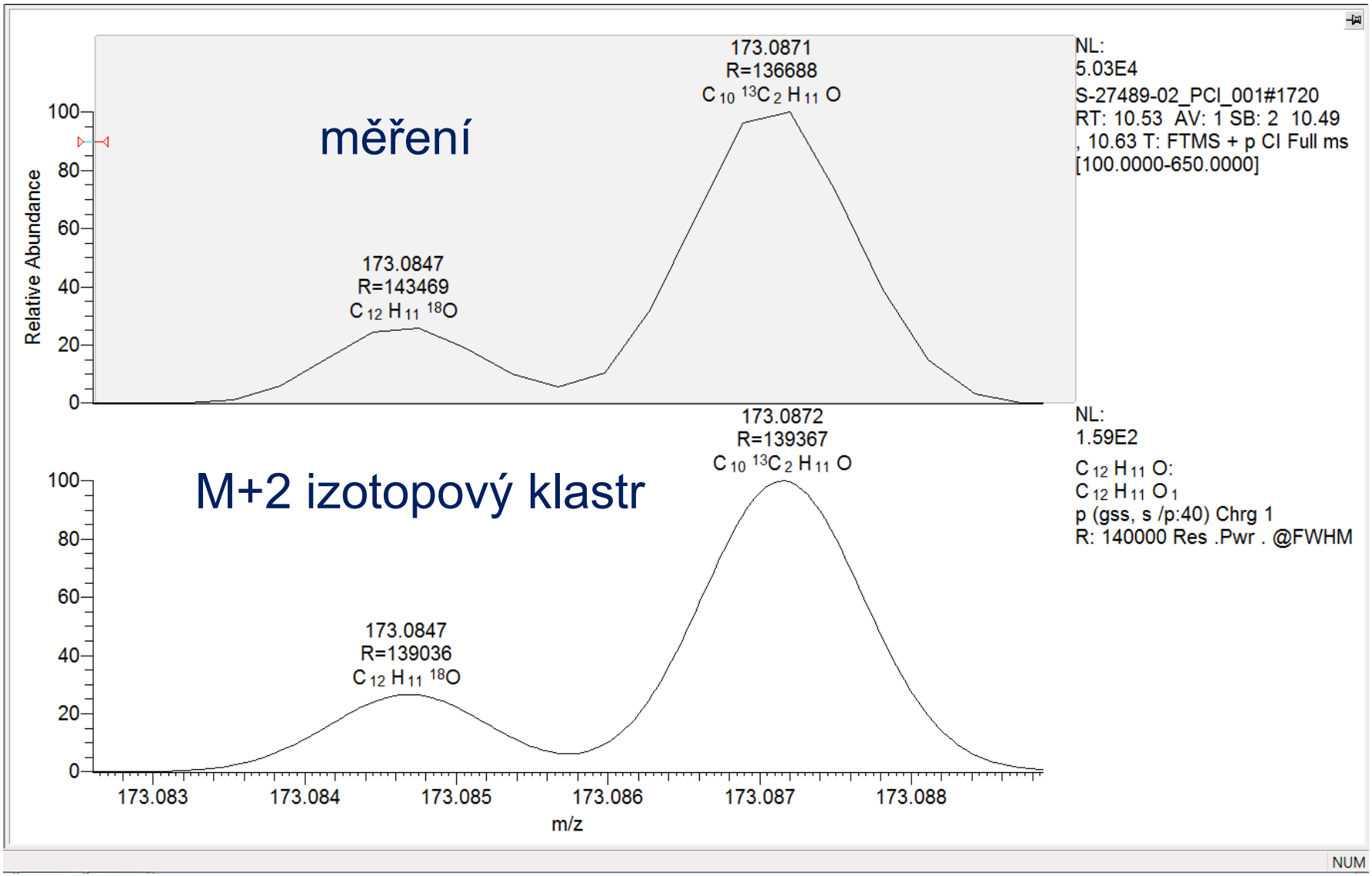
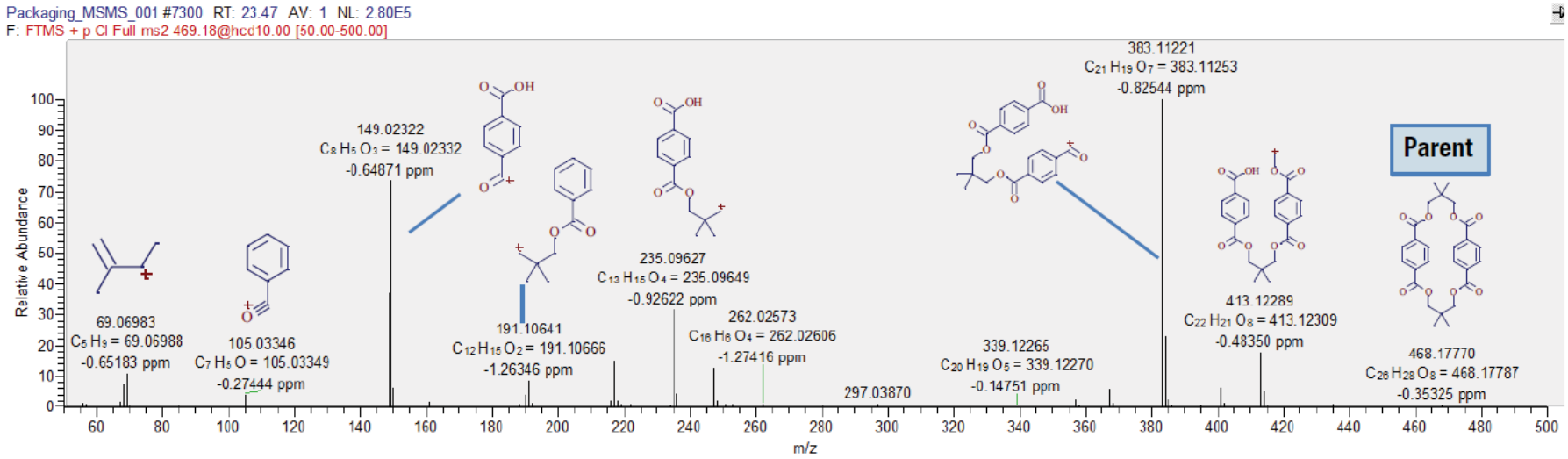
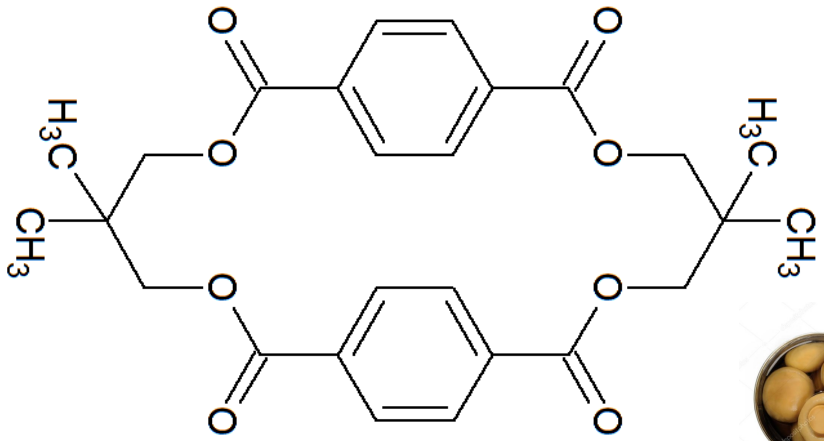
Identifikace



Identifikace – přehled





Compound Discoverer 2.0

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Děkuji za pozornost!

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