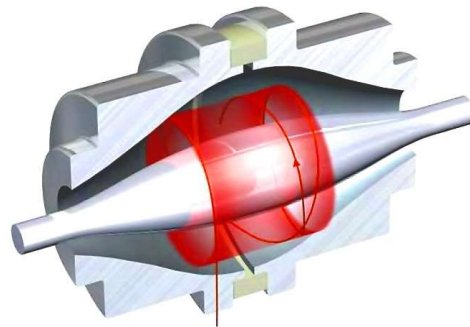


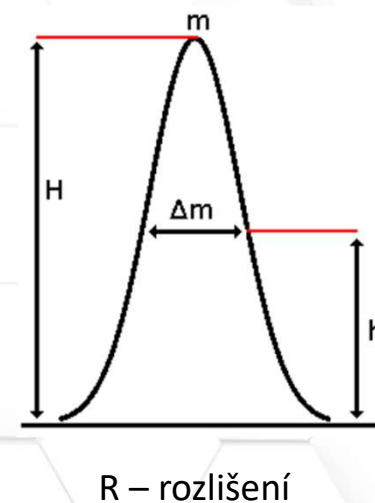
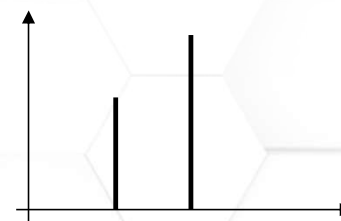
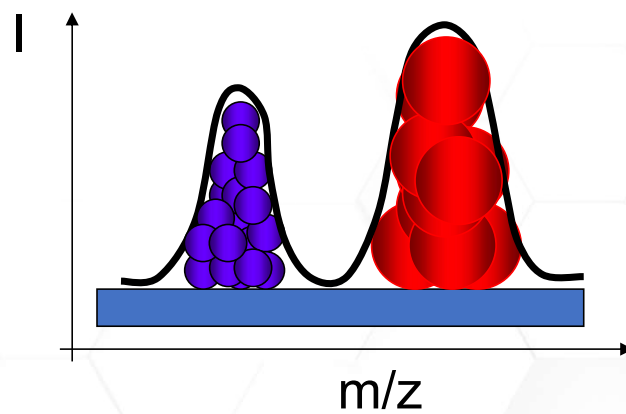
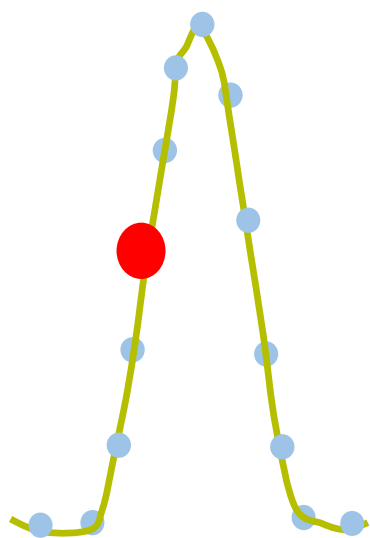
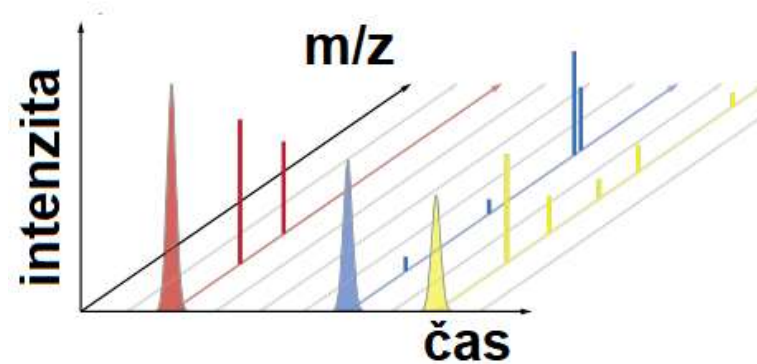
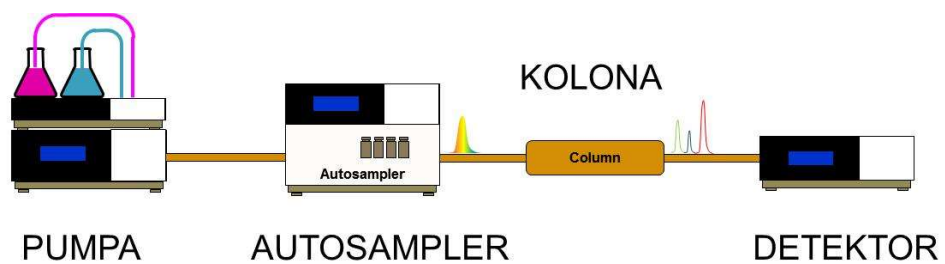


Dechberoucí vysoké rozlišení v hmotnostní spektrometrii

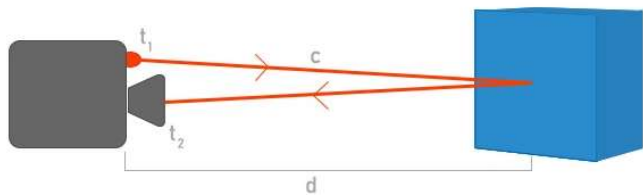
Lukáš Plaček



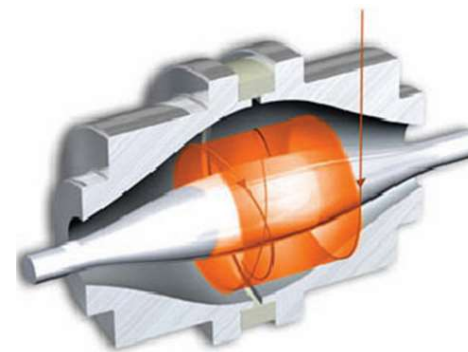
Hmotnostní spektrum



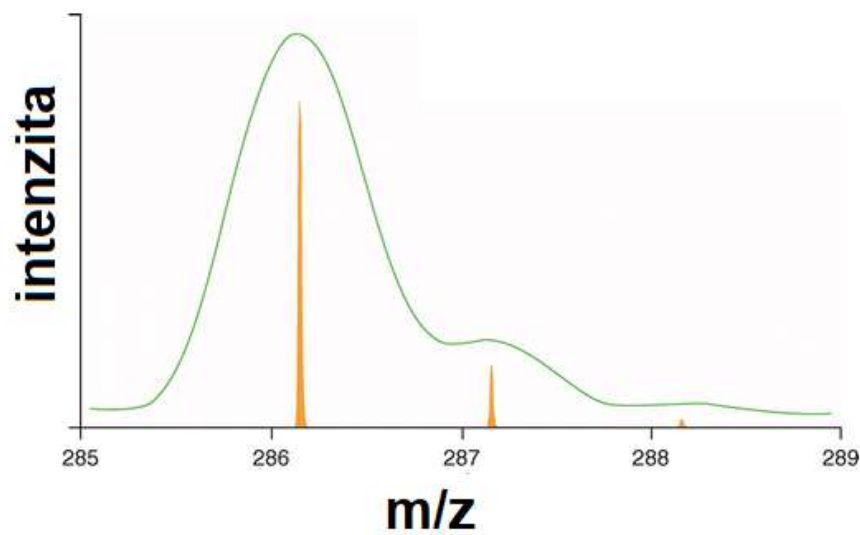
Moderní HRMS



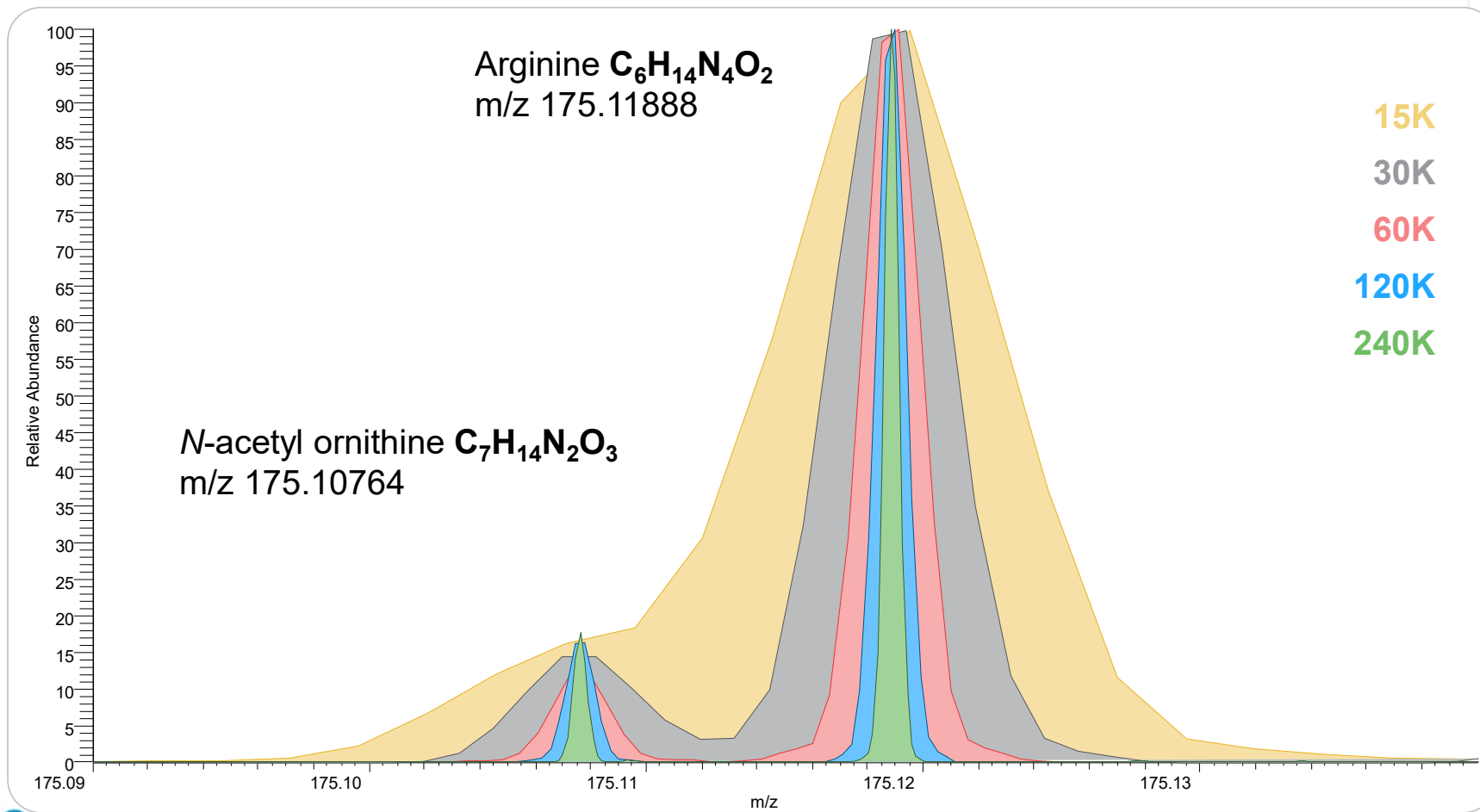
TIME OF FLIGHT (1946)

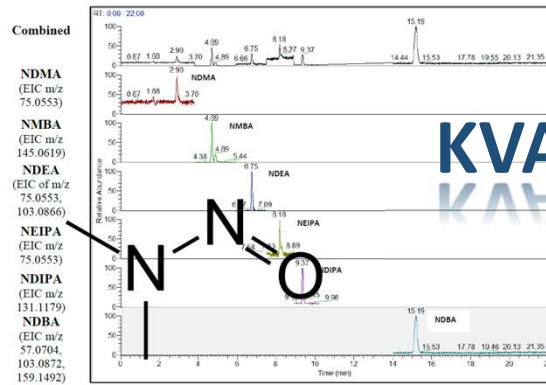


ORBITAL TRAP (2000)

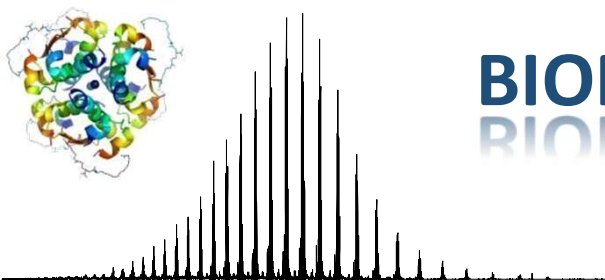


Proč vysoké rozlišení?

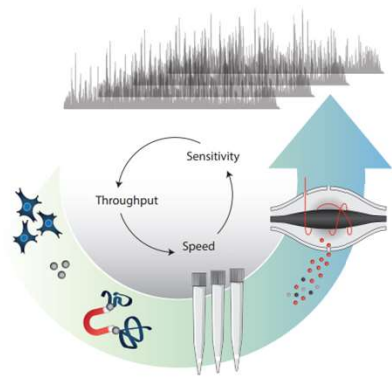




KVANTITA

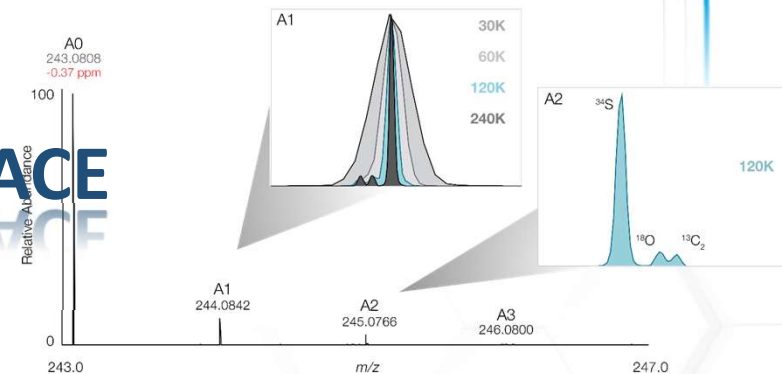


BIOPHARMA

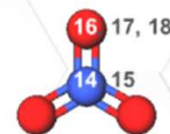
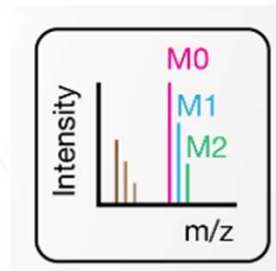


PROTEOMIKA

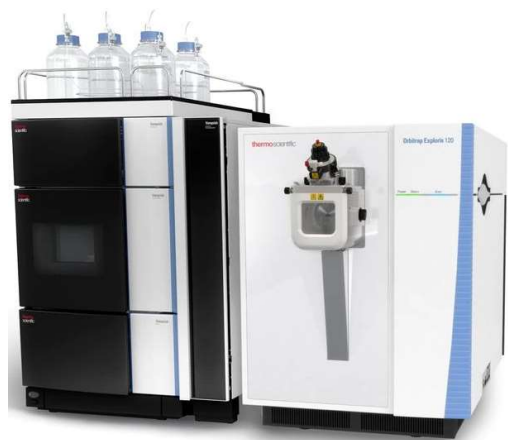
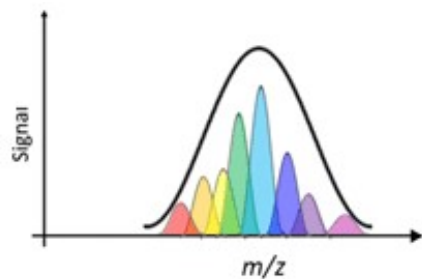
IDENTIFIKACE



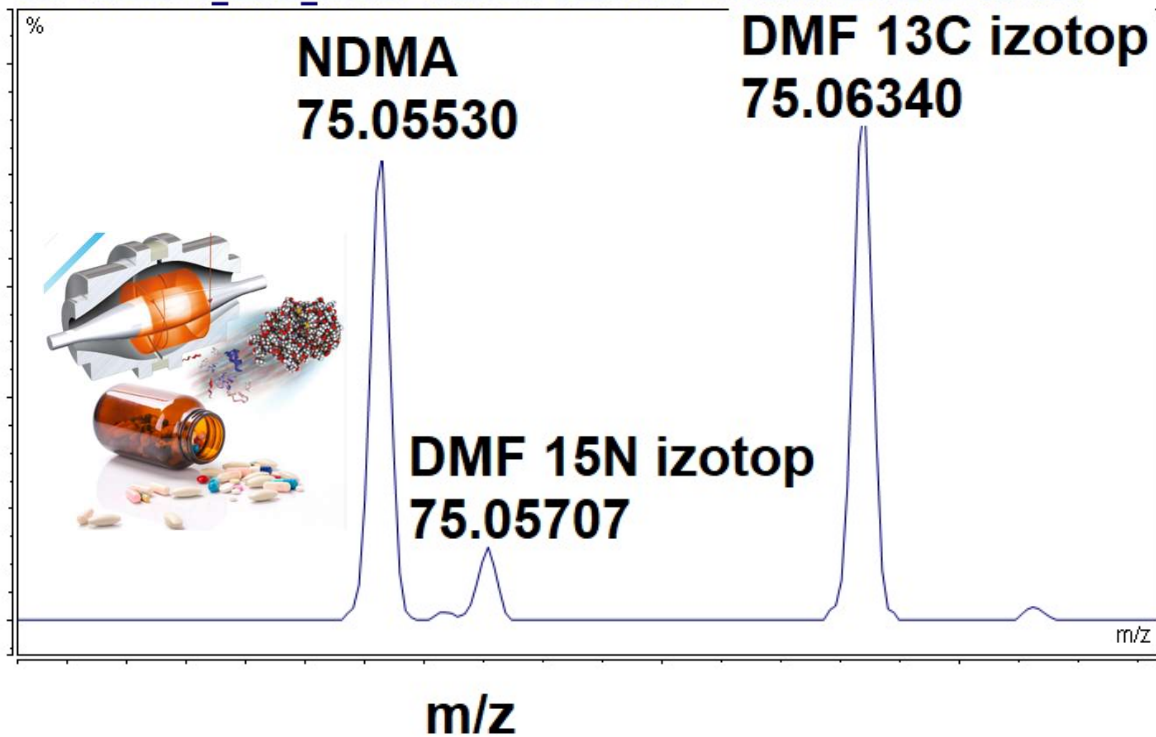
POMĚRY IZOTOPŮ

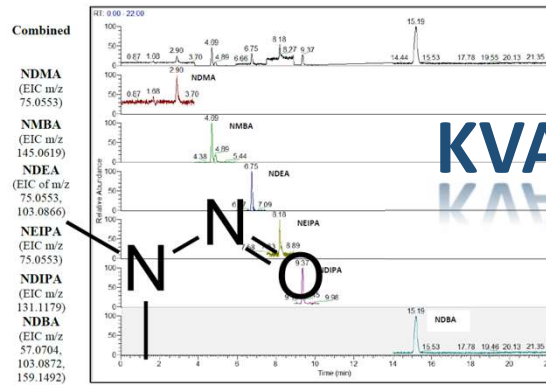


Kvantitativní HRMS

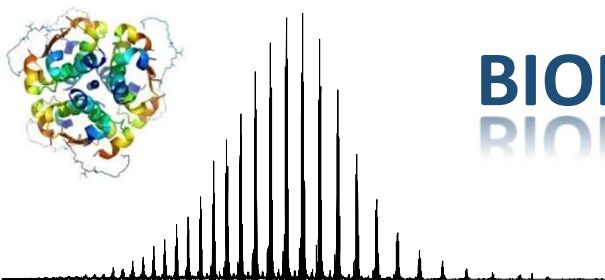


#51 Ranitidine_tablet_extract - Baseline Scan: #99 RT: 0.80 min NL: 3.49E+005

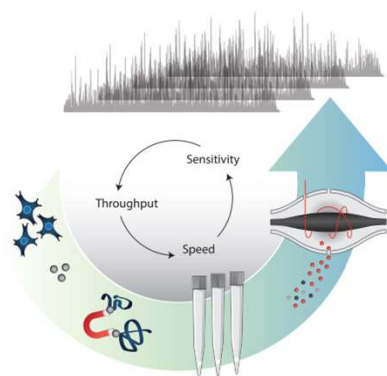




KVANTITA

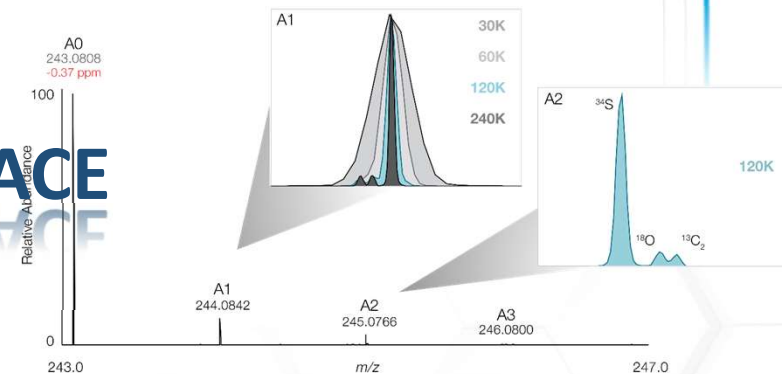


BIOPHARMA

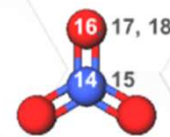
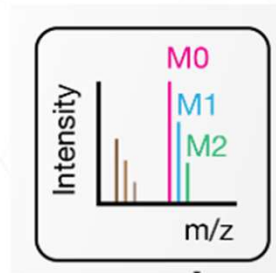


PROTEOMIKA

IDENTIFIKACE

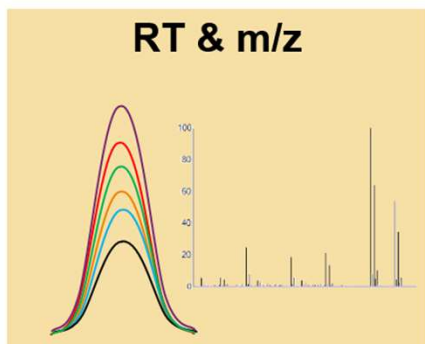


POMĚRY IZOTOPŮ



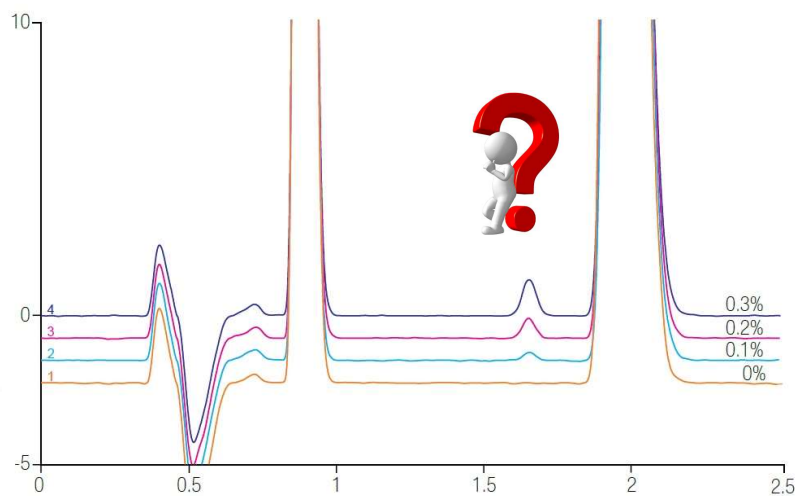
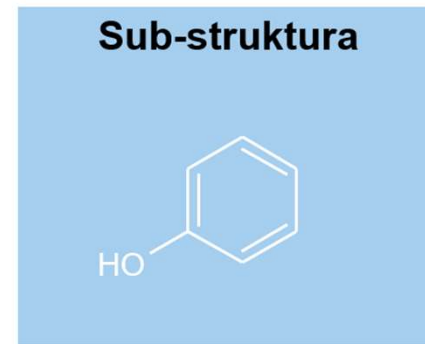
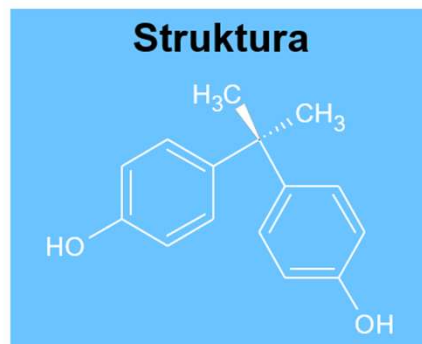


Identifikace látek



Elementární složení

$C_{15}H_{16}O_2$

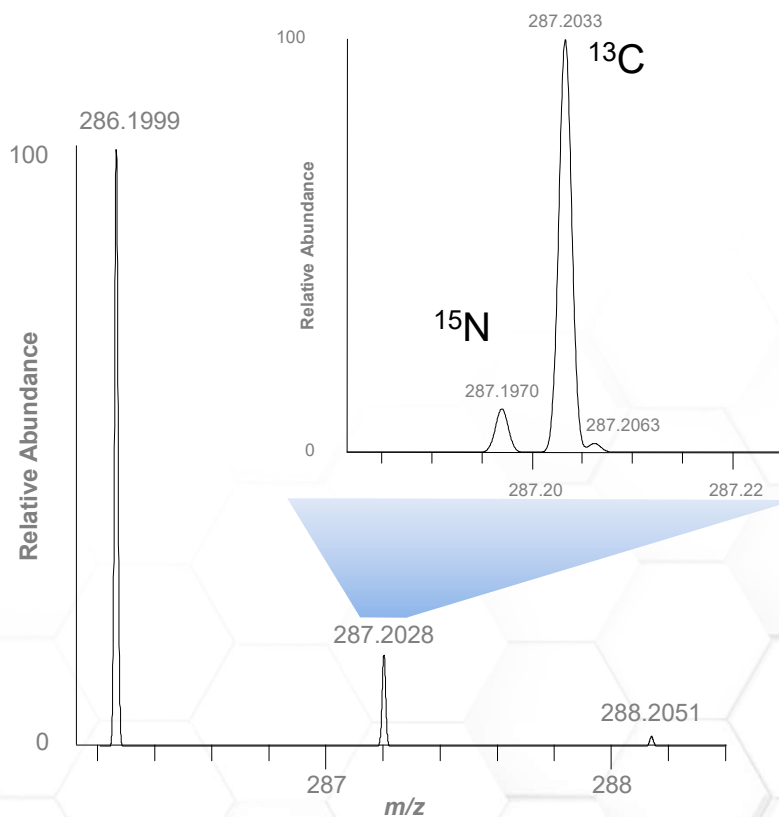




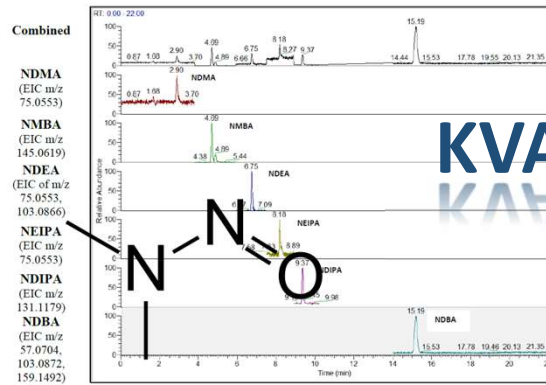
or



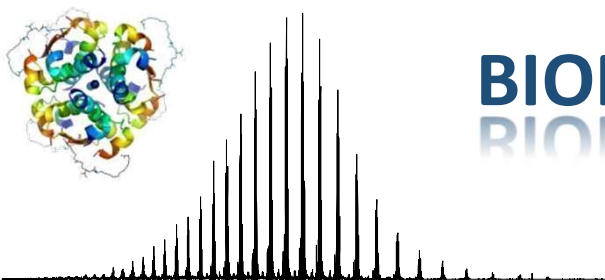
- přesná hmota a popis fragmentů nejsou jediné nástroje
- přesná hmota vede k elementárnímu složení
- velmi vysoké rozlišení značně pomůže ke zpřesnění elementárního složení



HRAM

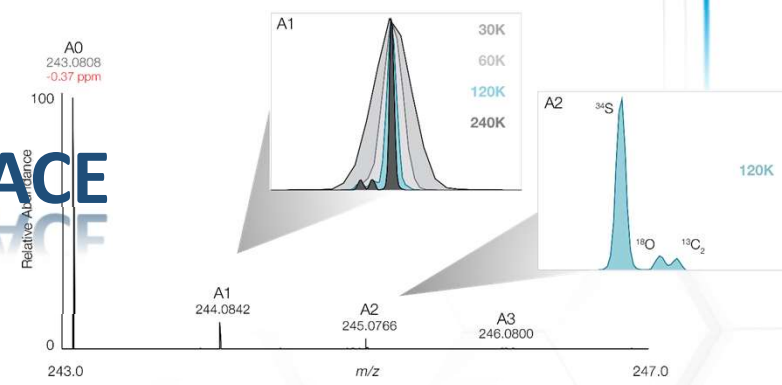


KVANTITA

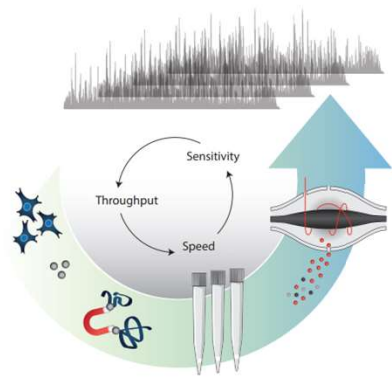
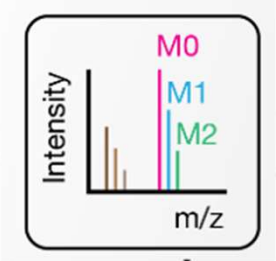


BIOPHARMA

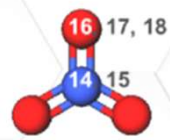
IDENTIFIKACE



POMĚRY IZOTOPŮ

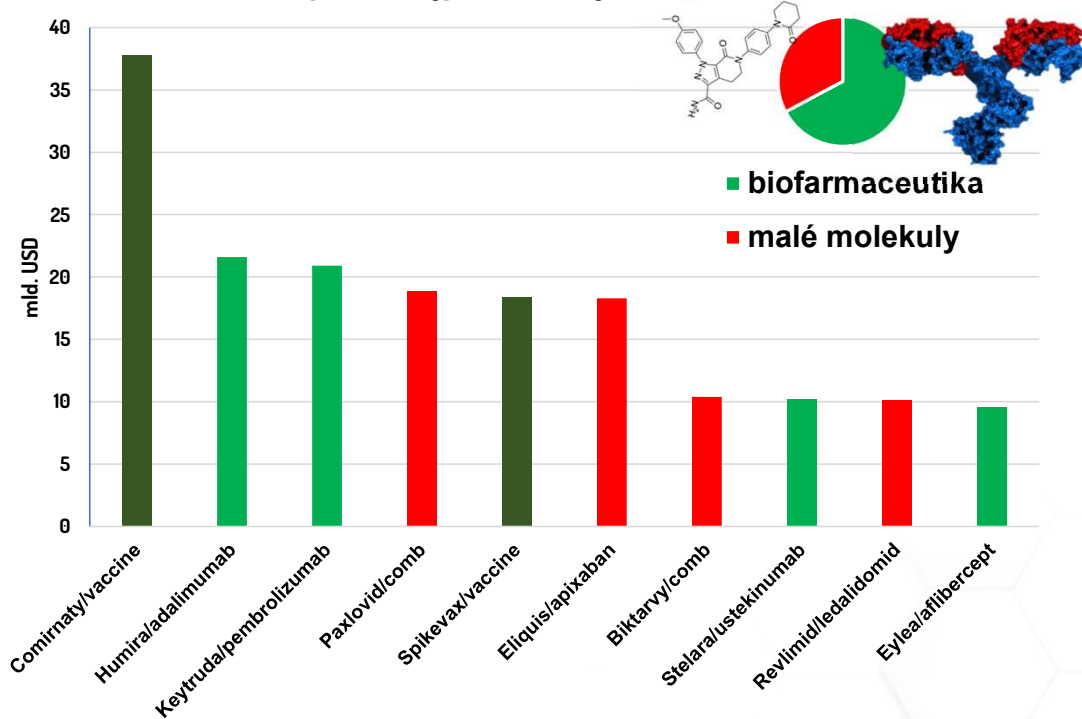


PROTEOMIKA

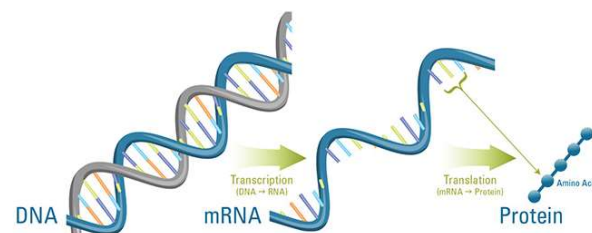
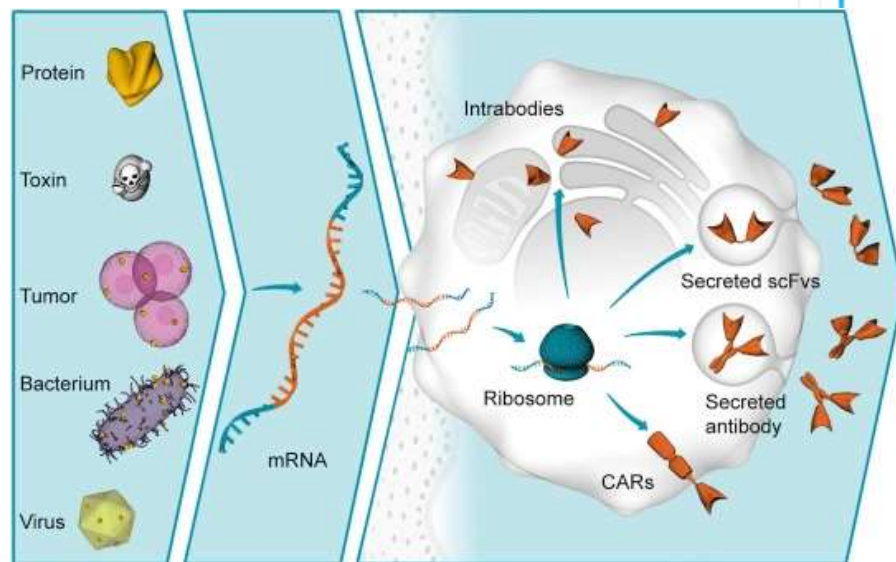


Trendy ve farmacii

Top 10 - nejprodávanější léky 2022



www.pharmacompass.com, www.genetherapy.isth.org



SAVE THE DATE

Hmotnostní spektrometrie v (bio)farmaceutické analýze

Mass Spectrometry in (Bio)Pharmaceutical Analysis

Datum:

28. 11. 2023

Místo:

Hotel Don Giovanni Prague

Přednášející:

prof. PharmDr. Lucie Nováková, Ph.D.

Farmaceutická fakulta v Hradci Králové, Univerzita Karlova

Mgr. Eva Harazim, Ph.D.

Teva Czech Industries s.r.o.

Ing. Michal Godula, Ph.D.

Thermo Fisher Scientific

Mgr. Martin Hubálek, Ph.D.

Ústav organické chemie a biochemie AV ČR, v. v. i.

Ing. Martina Čumová, Ph.D.

Synthon, s.r.o.

Ing. Lenka Svobodová, Ph.D.

APIGENEX s.r.o.

Ing. Matěj Šimek, Ph.D.

Contipro a.s.

Ing. Martin Moos, Ph.D.

Biologické centrum AV ČR, v. v. i.

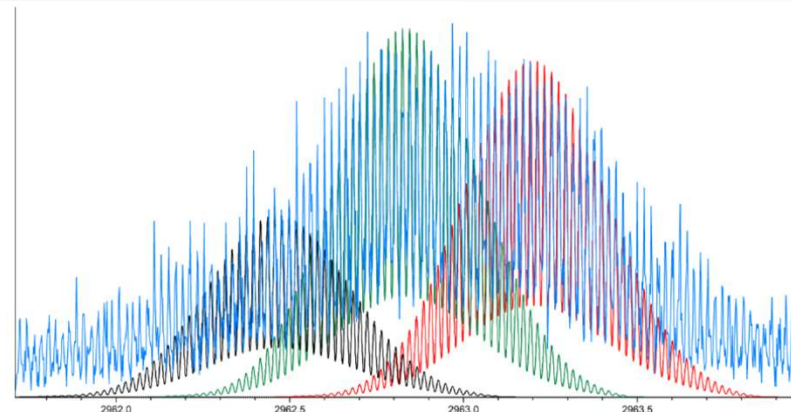
a další

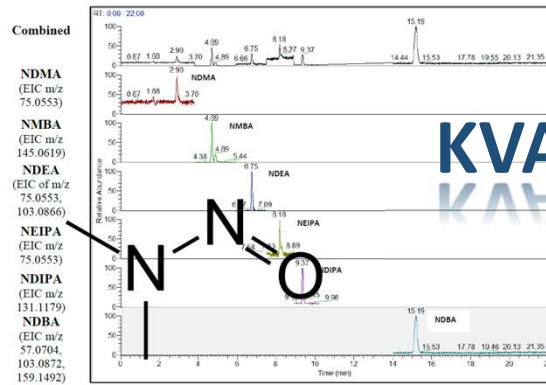
Datum:

28. 11. 2023

Místo:

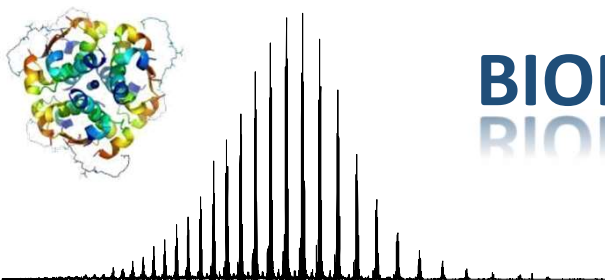
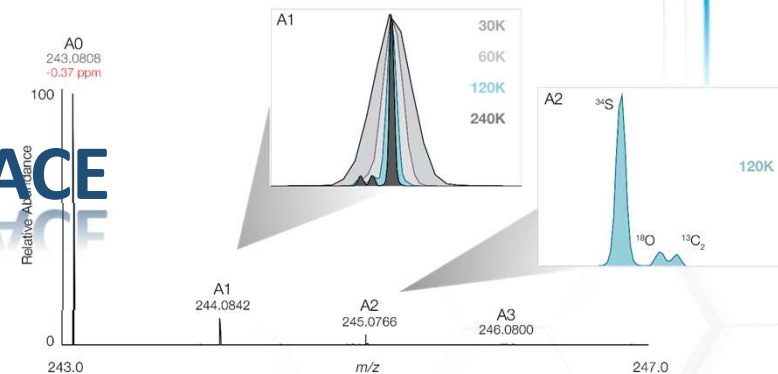
Hotel Don Giovanni Prague





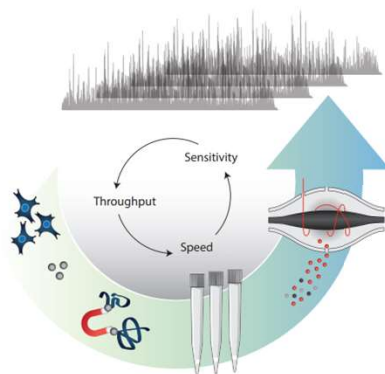
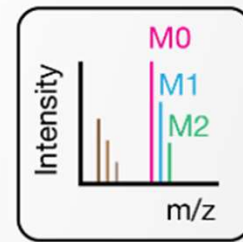
KVANTITA

IDENTIFIKACE

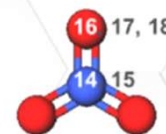


BIOPHARMA

POMĚRY IZOTOPŮ



PROTEOMIKA



IRMS: Isotope-ratio Mass Spectrometry

Periodic Table of Elements

C Carbon 6

Mass: 12.0107

Valence: 4

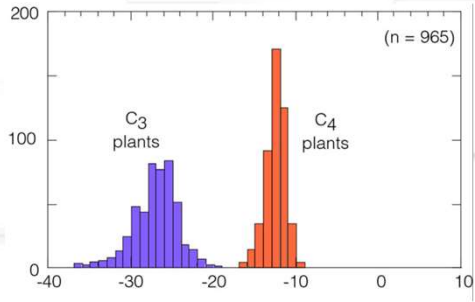
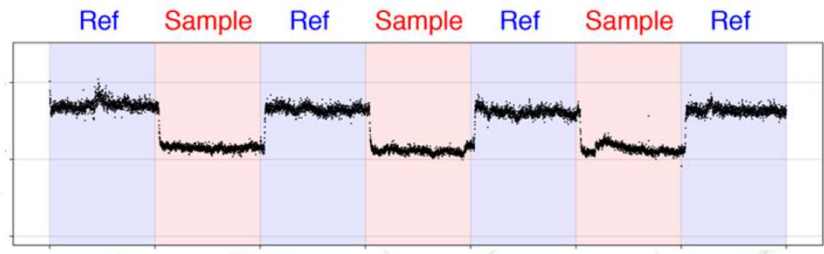
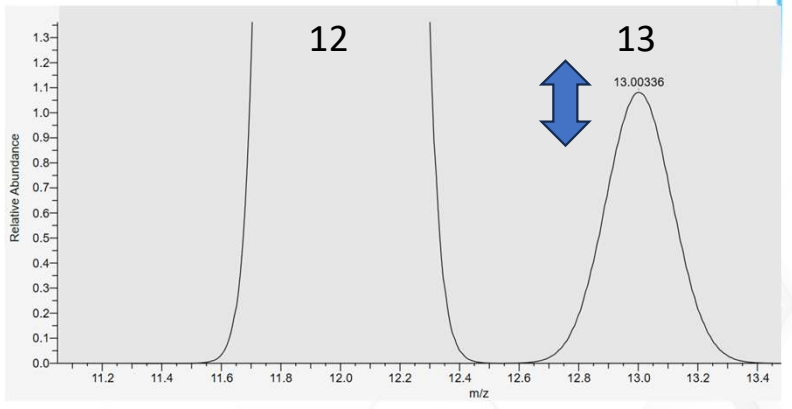
Electron configuration: 2-4

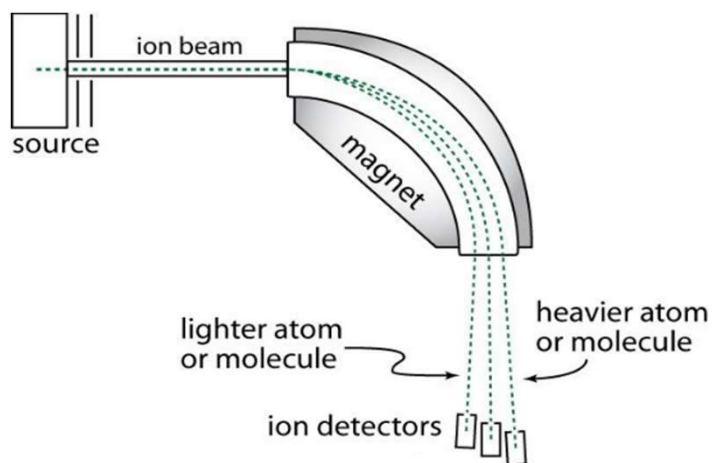
1	2											13	14	15	16	17	18	
H	He											B	C	N	O	F	Ne	
Li	Be											Al	Si	P	S	Cl	Ar	
Na	Mg	3	4	5	6	7	8	9	10	11	12	Ga	Ge	As	Se	Br	Kr	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	In	Sn	Sb	Te	I	Xe	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	Hg	Tl	Pb	Bi	Po	At	Rn
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og	

* La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu D

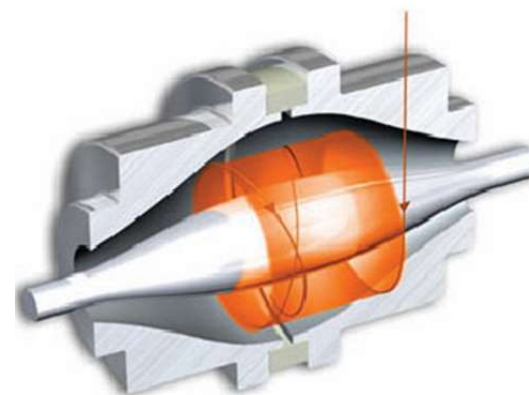
** Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr T

Isotope	%	Mass	Isotope	%	Mass	Isotope	%	Mass
12	98.9	12						
13	1.1	13.00335483						
[14]	0	14.003241						

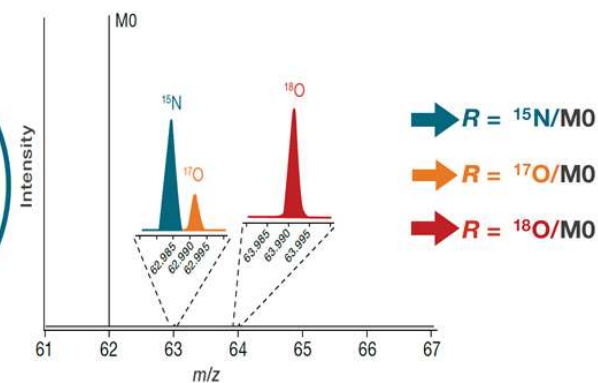
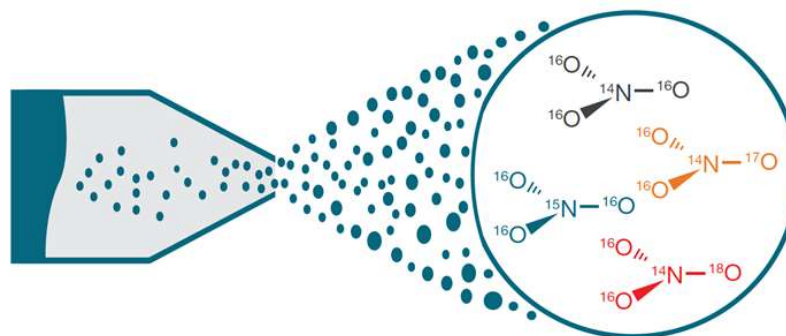
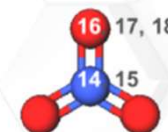




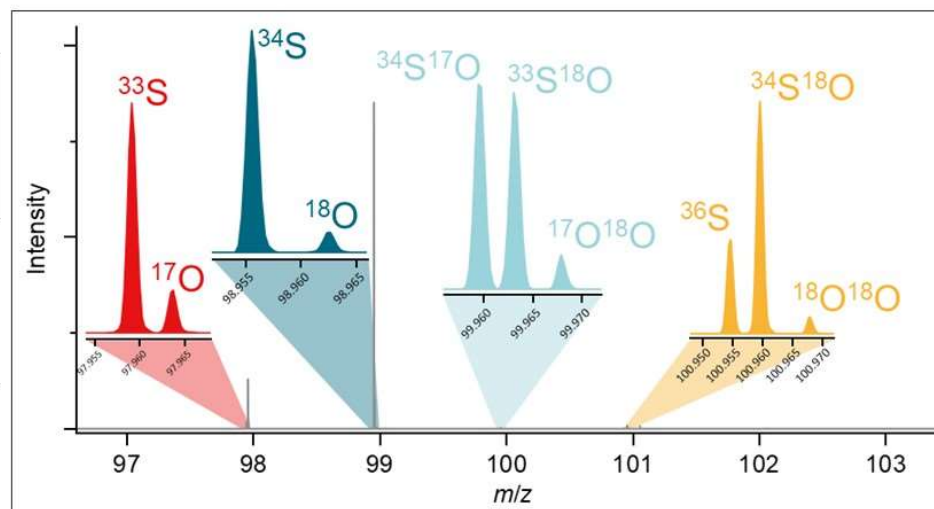
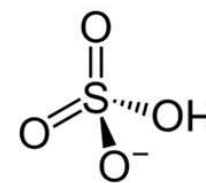
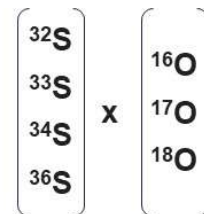
Classic isotope-ratio MS (CO_2 , N_2 , O_2 ,...)



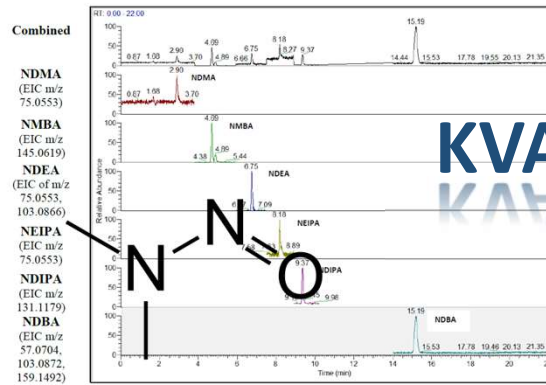
Thermo Scientific Orbitrap™ MS



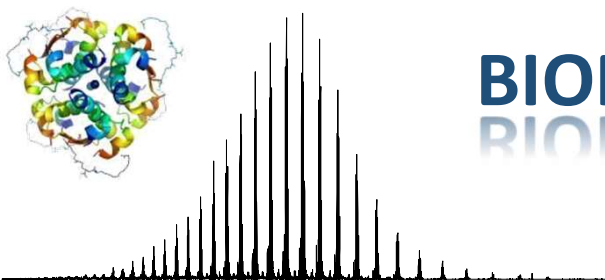
	<i>m/z</i>	Isotopologue	Abundance
M0	96.9596	$^1\text{H}^{32}\text{S}^{16}\text{O}_4$	9408592
M+1	97.9590	$^1\text{H}^{33}\text{S}^{16}\text{O}_4$	7427
	97.9638	$^1\text{H}^{32}\text{S}^{17}\text{O}^{16}\text{O}_3$	1433
M+2	98.9554	$^1\text{H}^{34}\text{S}^{16}\text{O}_4$	42084
	98.9638	$^1\text{H}^{32}\text{S}^{18}\text{O}^{16}\text{O}_3$	7632
M+3	99.9596	$^1\text{H}^{34}\text{S}^{17}\text{O}^{16}\text{O}_3$	63
	99.9632	$^1\text{H}^{33}\text{S}^{18}\text{O}^{16}\text{O}_3$	59
	99.9680	$^1\text{H}^{32}\text{S}^{17}\text{O}^{18}\text{O}^{16}\text{O}_2$	9
M+4	100.9546	$^1\text{H}^{36}\text{S}^{16}\text{O}_4$	145
	100.9596	$^1\text{H}^{34}\text{S}^{18}\text{O}^{16}\text{O}_3$	333
	100.9680	$^1\text{H}^{32}\text{S}^{18}\text{O}_2^{16}\text{O}_2$	44



Rozlišení R = 240 000

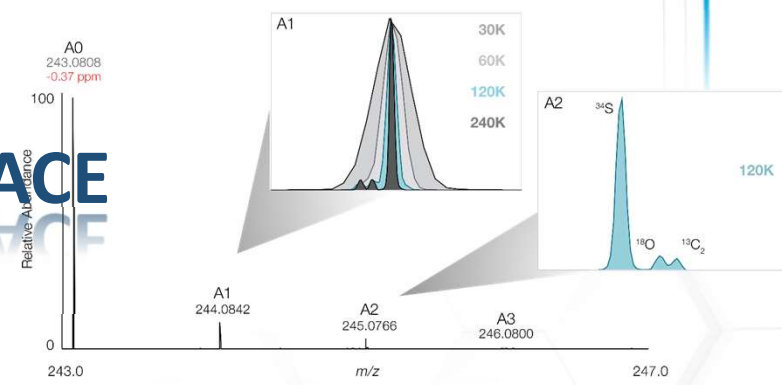


KVANTITA

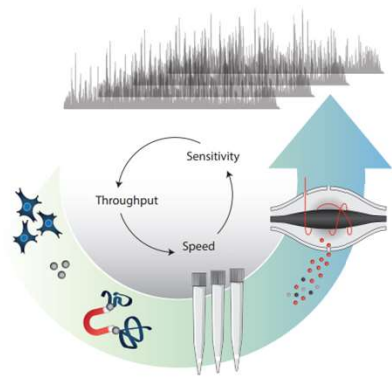
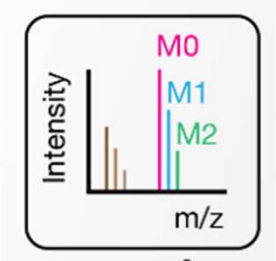


BIOPHARMA

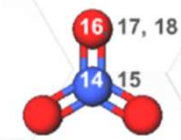
IDENTIFIKACE



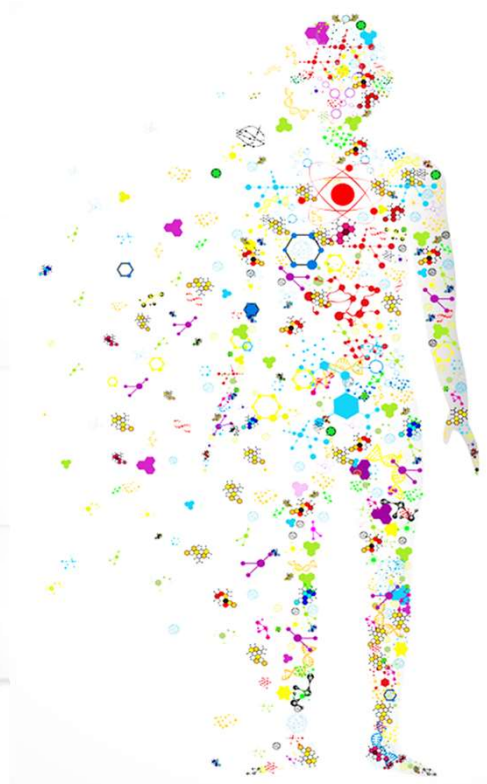
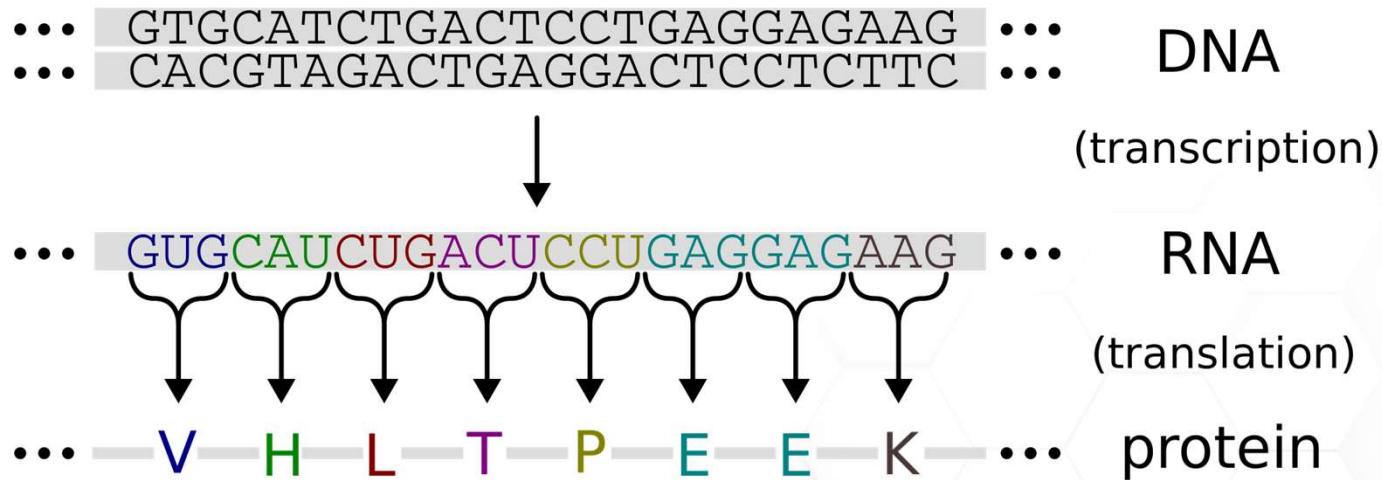
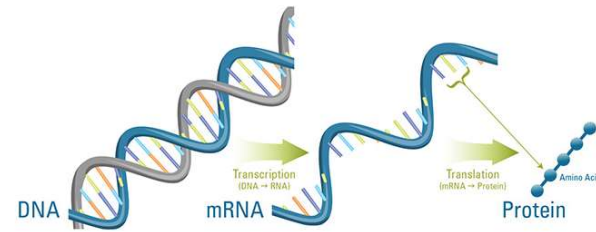
POMĚRY IZOTOPŮ



PROTEOMIKA

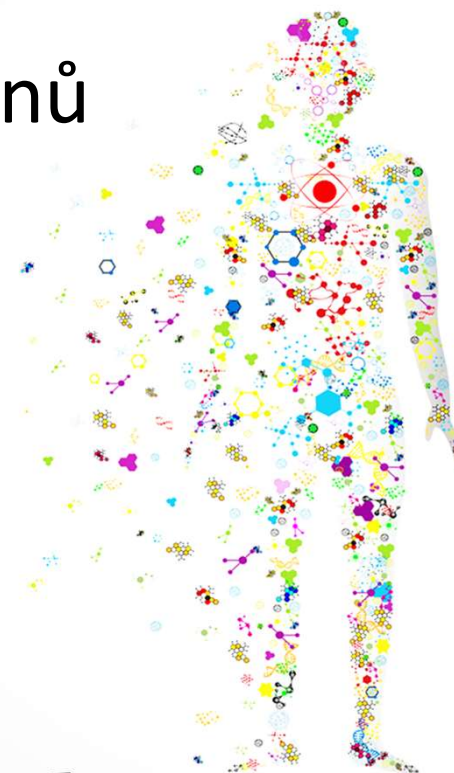
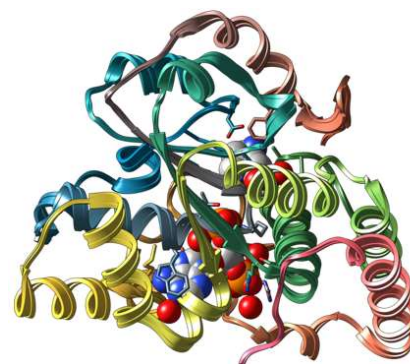
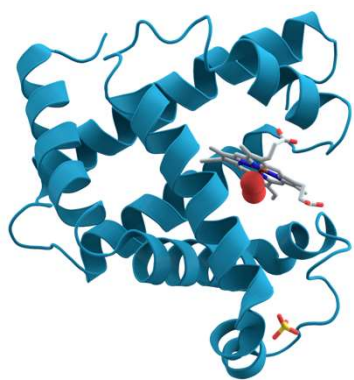


Proteomika



Lidský proteom

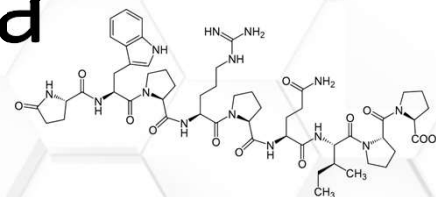
> **15 000** proteinů



~ 50 kDa → 50x 1kDa

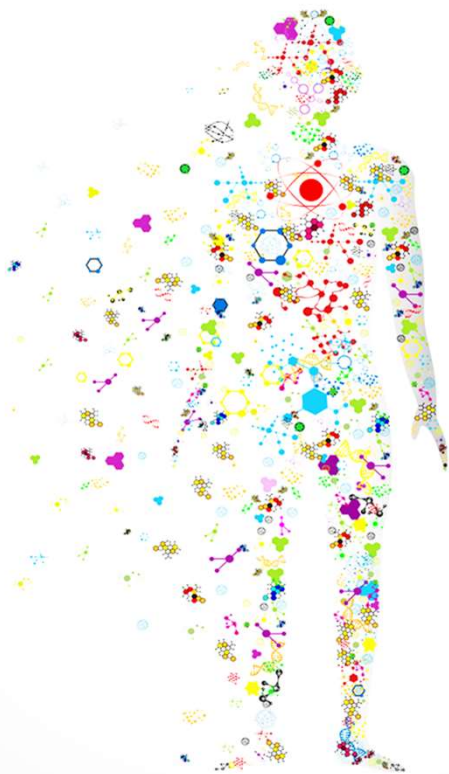
pragolab

Bottom-up proteomika

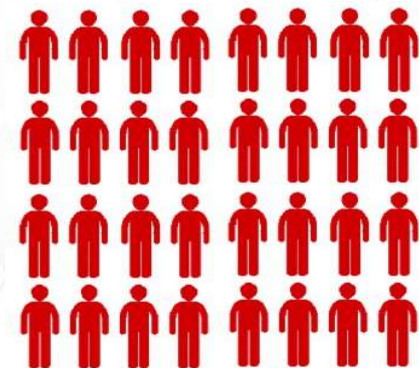
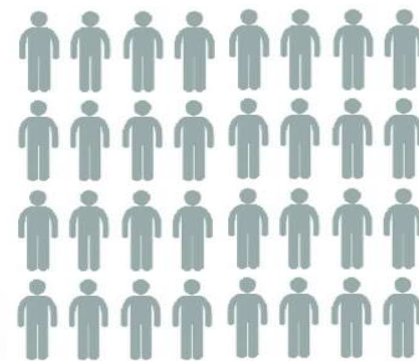
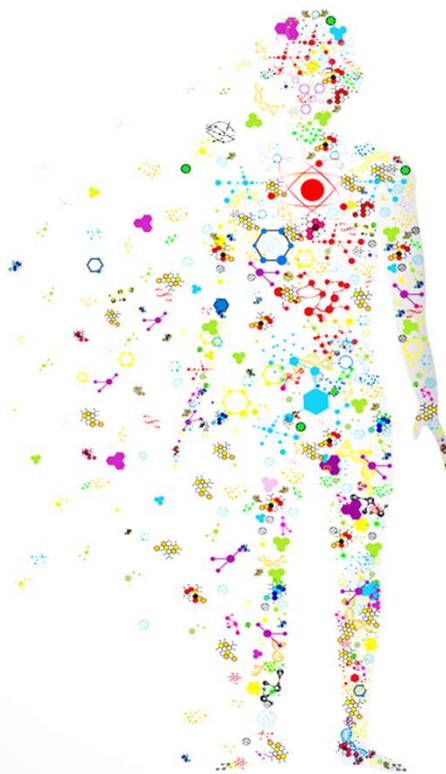


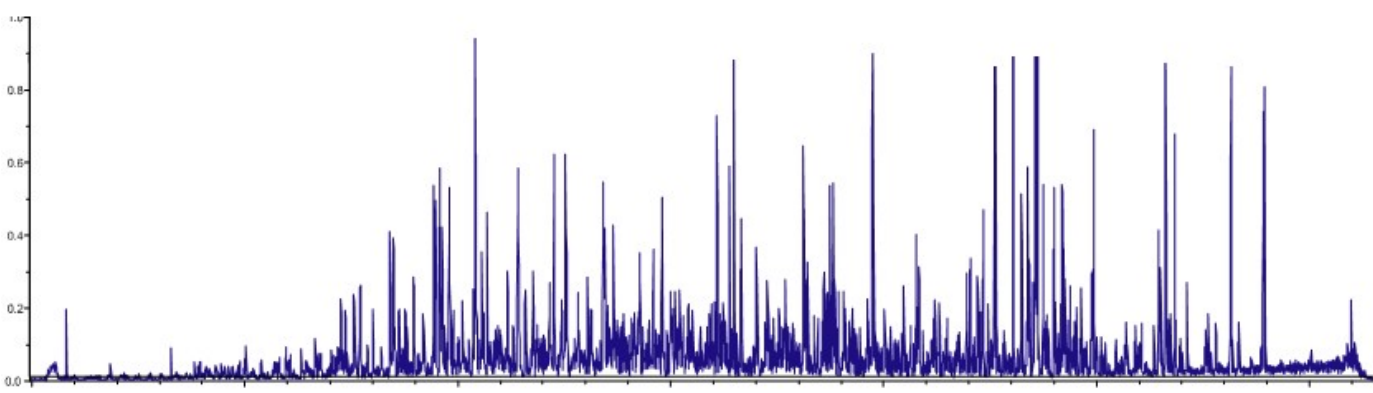
Hledání biomarkerů (jehličky v kupce sena)

zdravý



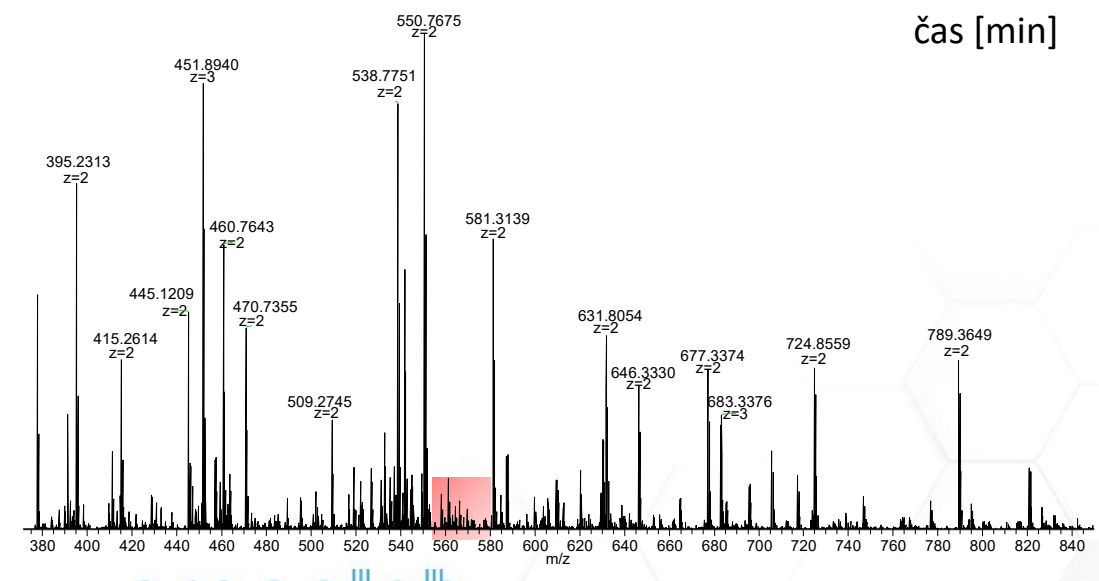
nemocný





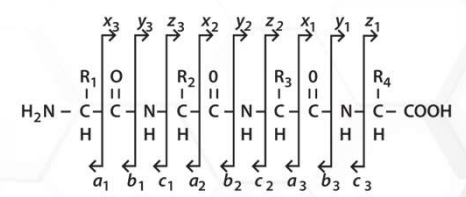
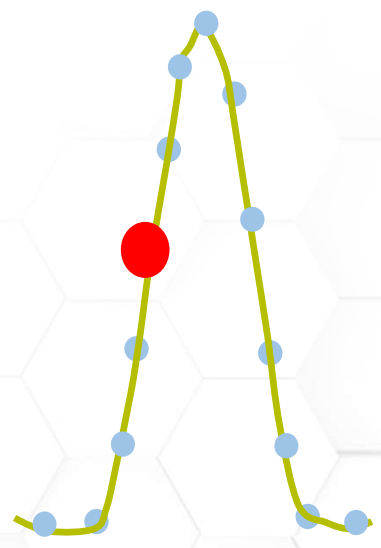
750 000 látek za 120 min
= cca 100 látek za sekundu

Potřeba 1x full scan HRMS
100 MS/MS (HRMS) za sekundu

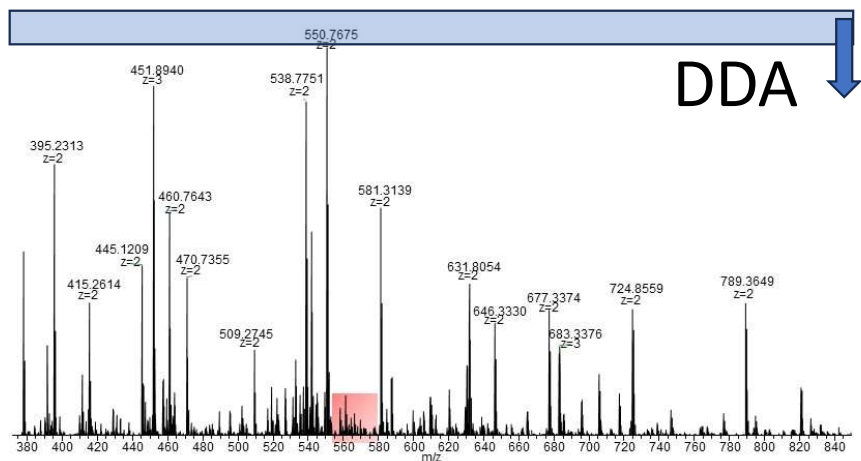


čas [min]

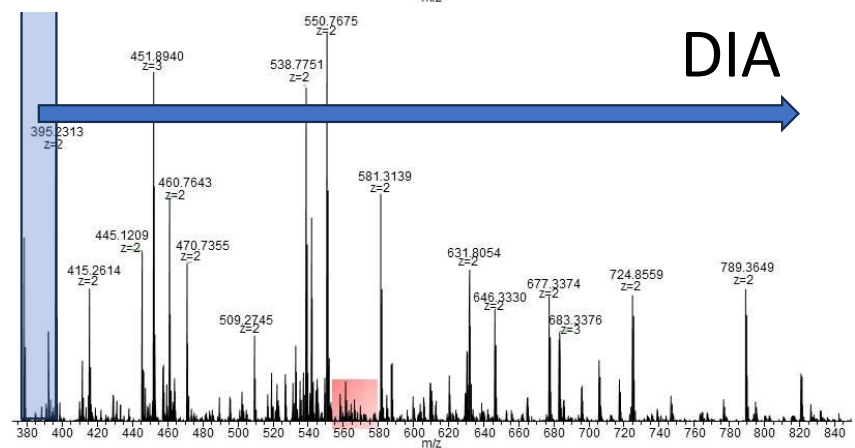
m/z



DDA vs. DIA

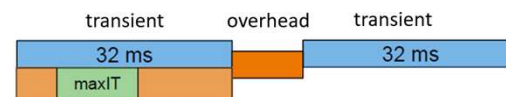


DDA ↓

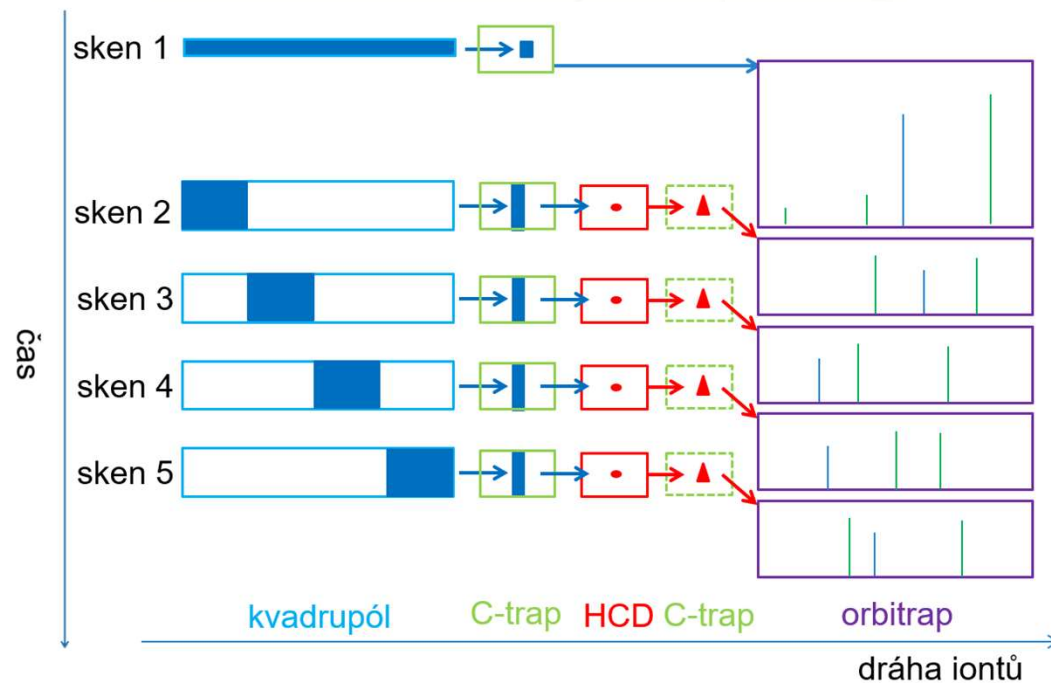


DIA →

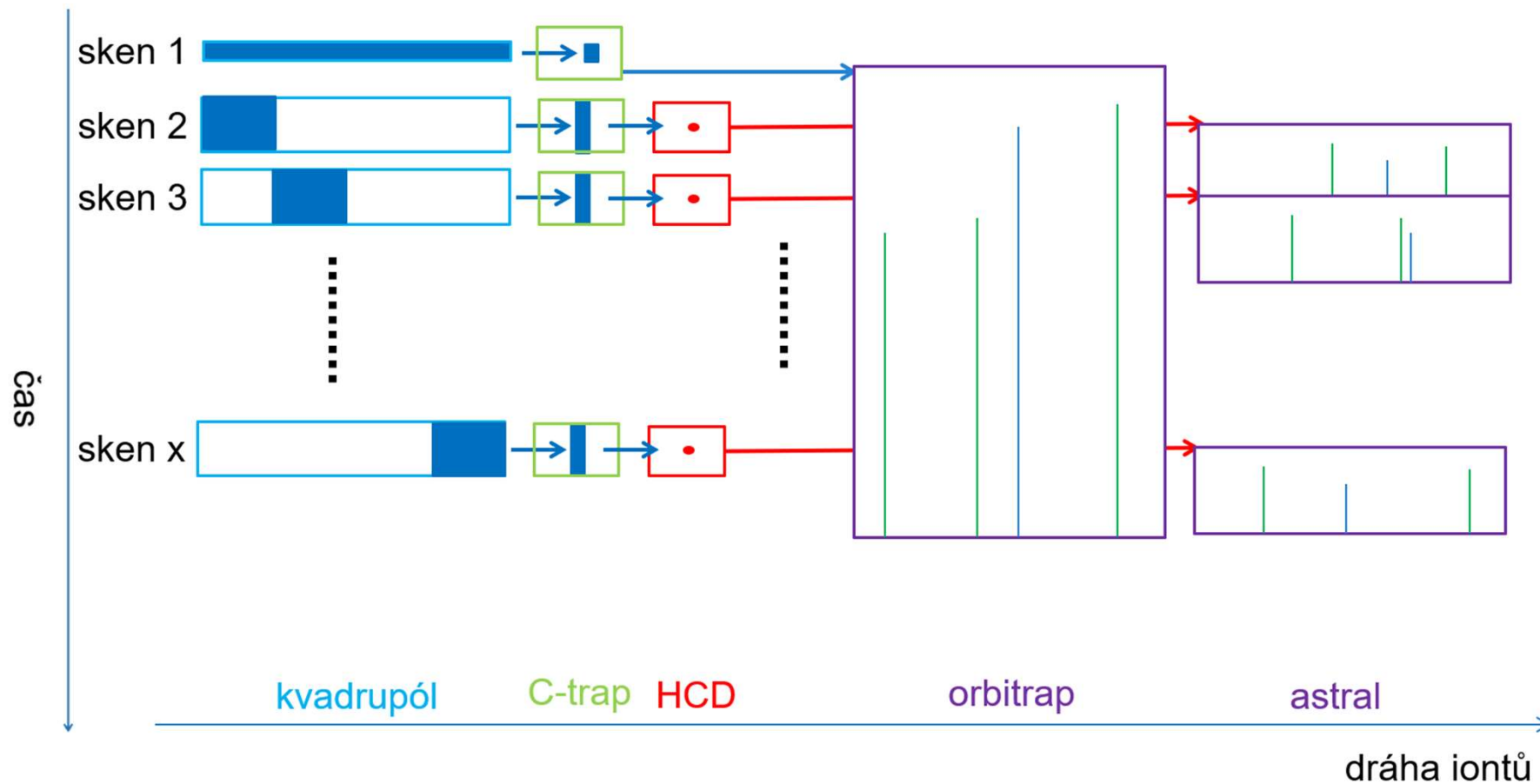
pragolab



rozlišení	transient	vzorkování
7 500	16 ms	40 Hz
15 000	32 ms	22 Hz
30 000	64 ms	12 Hz
60 000	128 ms	7 Hz
120 000	256 ms	3 Hz
240 000	512 ms	2 Hz
480 000	1024 ms	1 Hz



Orbitrap Astral

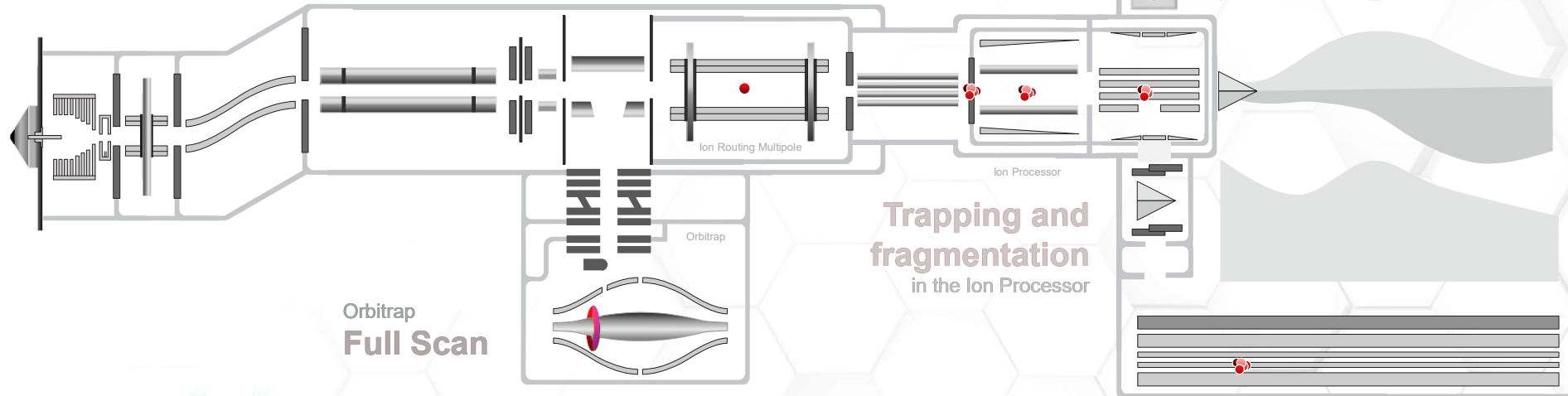
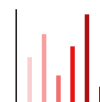


Orbitrap Astral



Ejection and scanning
in the Astral analyzer

Precursor range isolation
in Quadrupole and
ion concentration
in Ion Routing Multipole



Orbitrap
Full Scan

Ion Routing Multipole

Ion Processor

Trapping and fragmentation
in the Ion Processor

Astral Analyzer



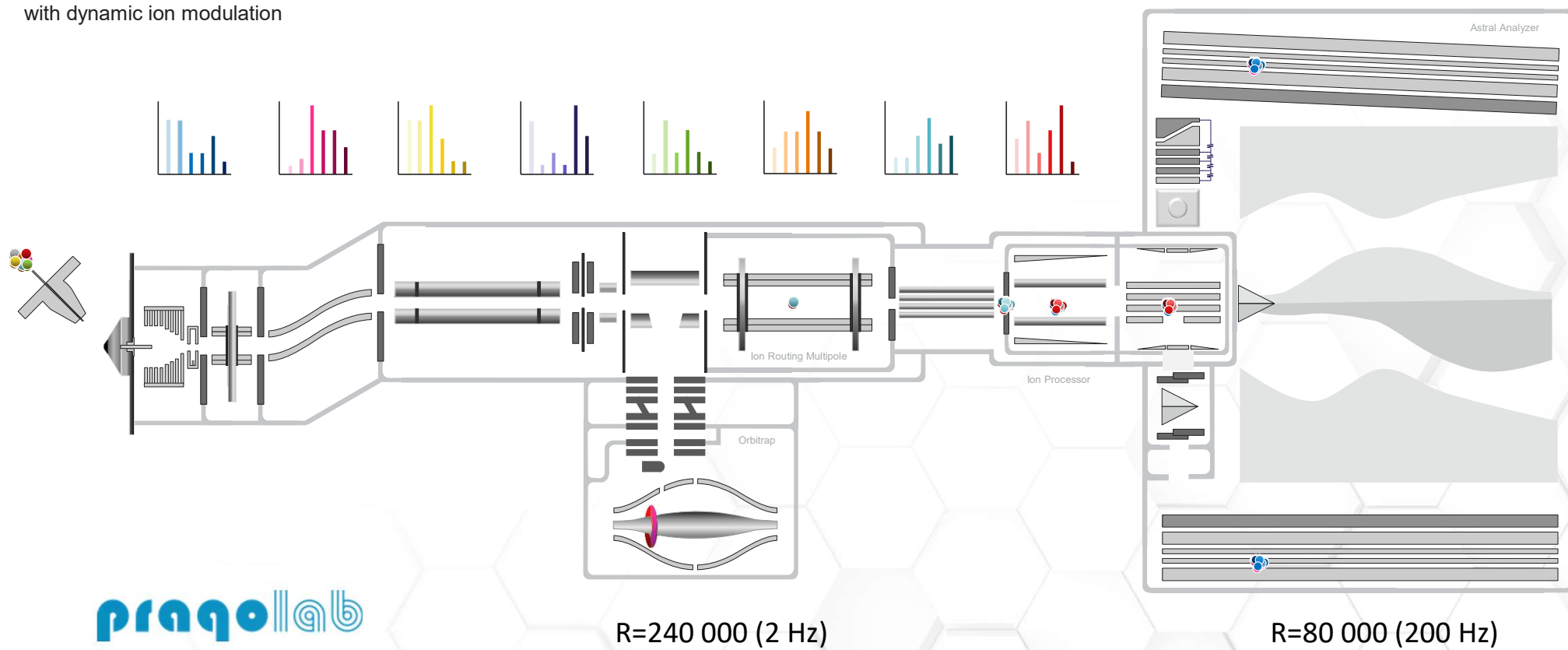
R=240 000 (2 Hz)

R=80 000 (200 Hz)

Orbitrap Astral

5 ion packets

simultaneously processed in parallel
with dynamic ion modulation





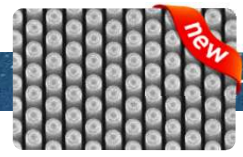
**Thermo Scientific™
AccelerOme™**
Automated
sample preparation



**Thermo Scientific™
Vanquish™ Neo
UHPLC system**
Chromatography



**Thermo Scientific™
μPAC Neo
columns**
Separation



**Thermo Scientific™
FAIMS Pro
Duo interface**
Gas phase separation



**Orbitrap
Astral MS**
Data acquisition



**Thermo Scientific™
Proteome Discoverer™
software
powered by Ardia™**
Data processing



The next generation proteomics workflow

An end-to-end solution for proteomics





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