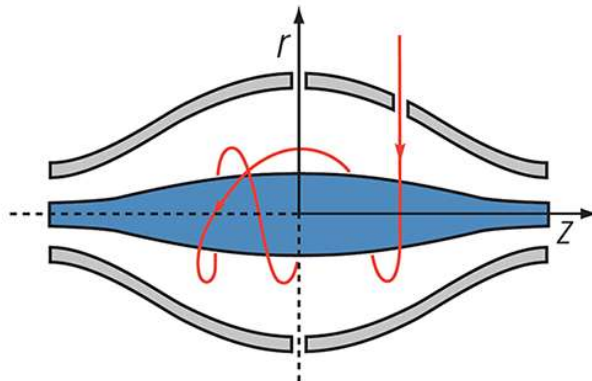




Historie, vývoj a progres orbitálních pastí

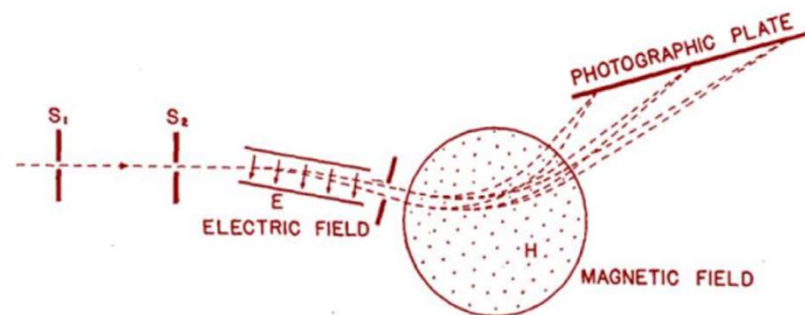
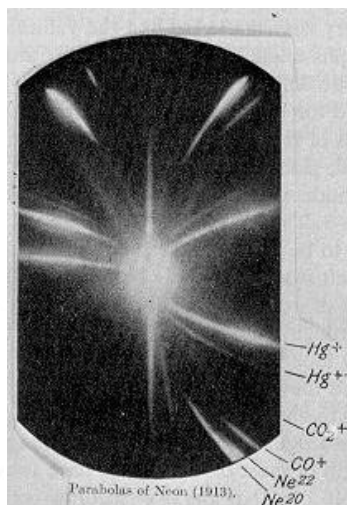
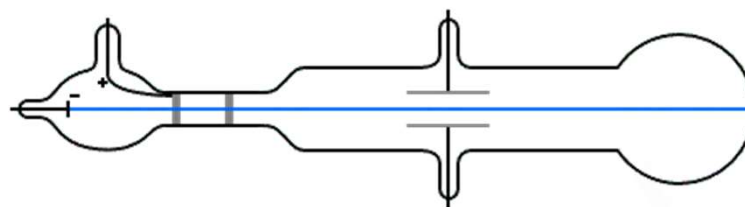
Lukáš Plaček



Počátky hmotnostní spektrometrie

J.J. Thomson (1897)

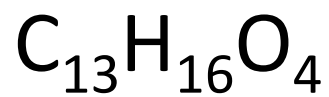
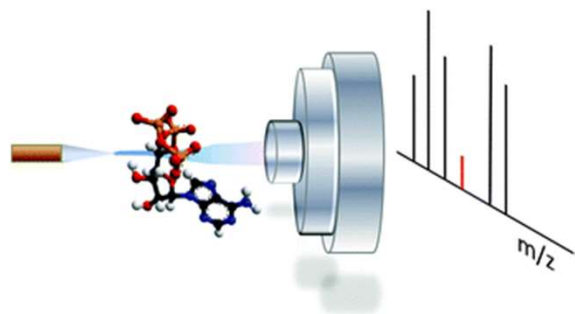
F. Aston (1919)



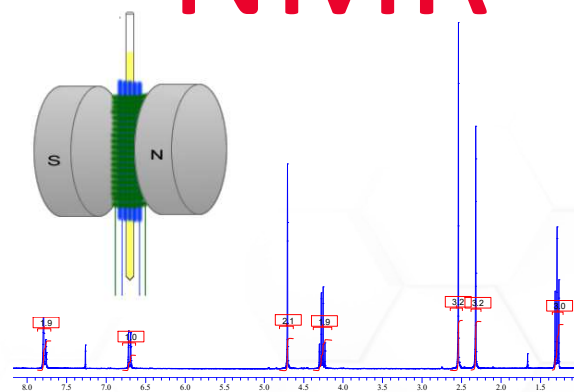
Ion optics of Aston's First Mass Spectrograph

Strukturní analýza

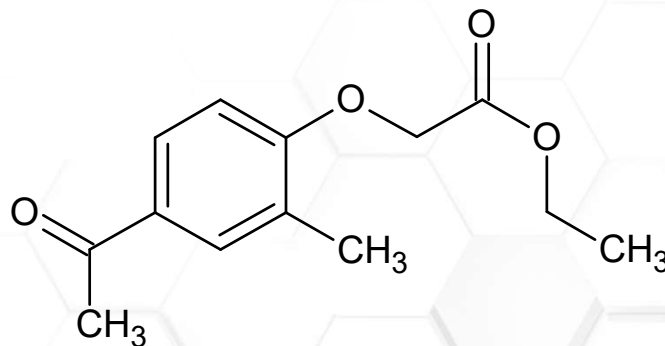
MS



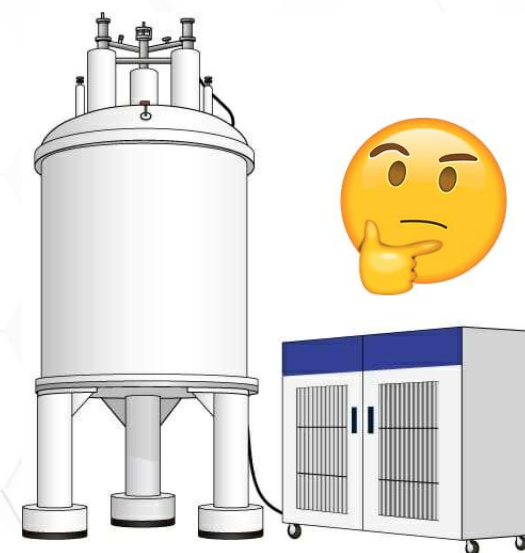
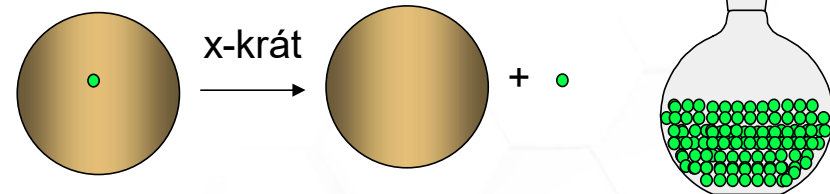
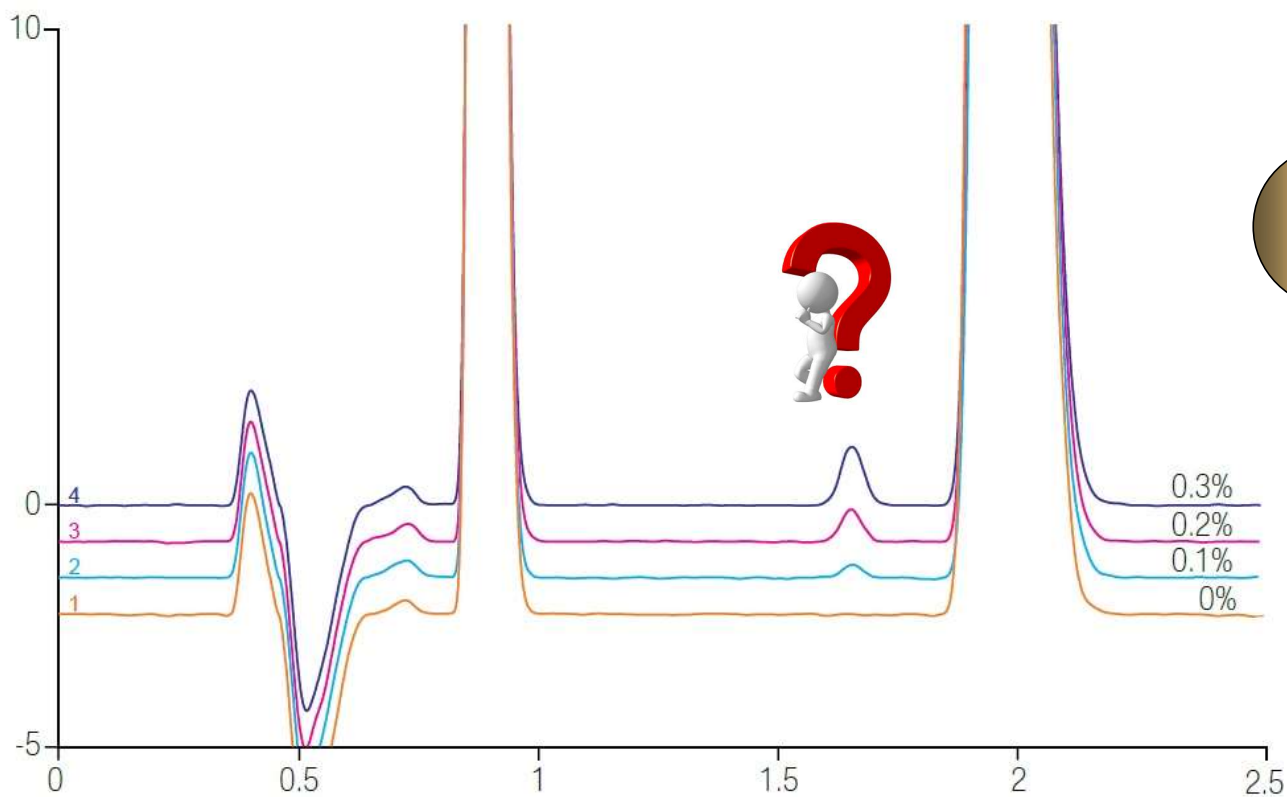
NMR



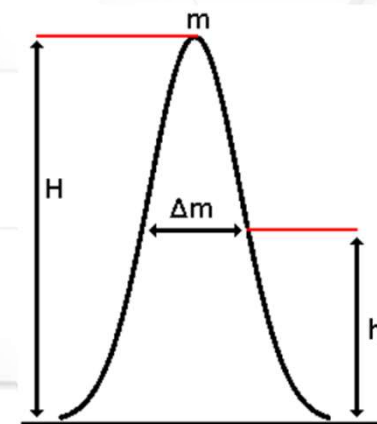
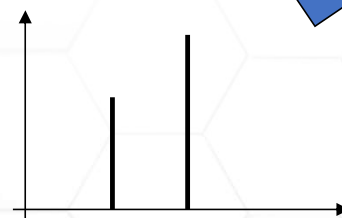
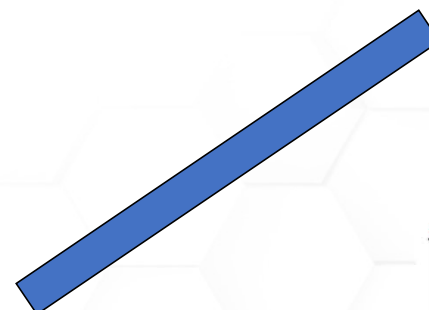
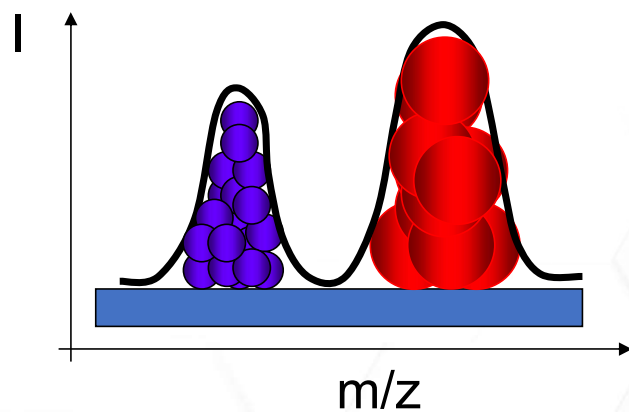
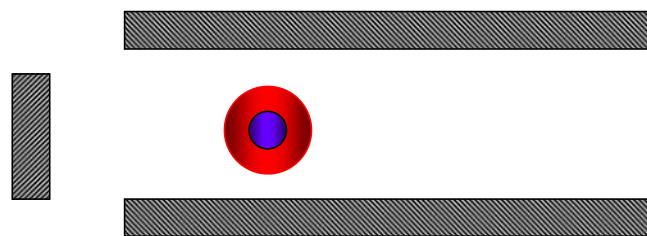
3x substituovaný Ar
3x CH_3 + 2x $\text{O}-\text{CH}_2-$
1x $\text{C}=\text{O}$ + 1x $\text{O}-\text{C}=\text{O}$



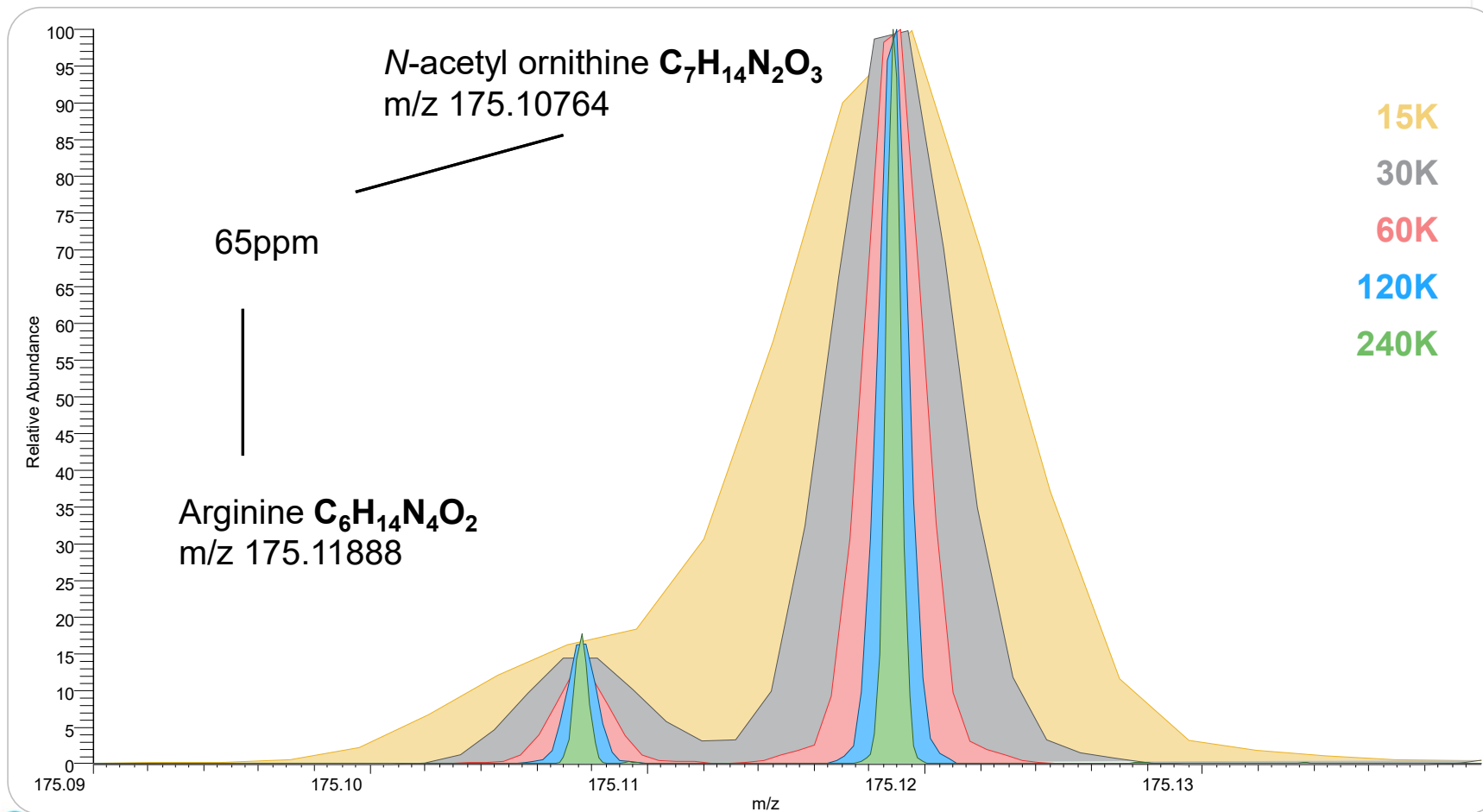
Strukturní analýza



Hmotnostní spektrum



Proč vysoké rozlišení?

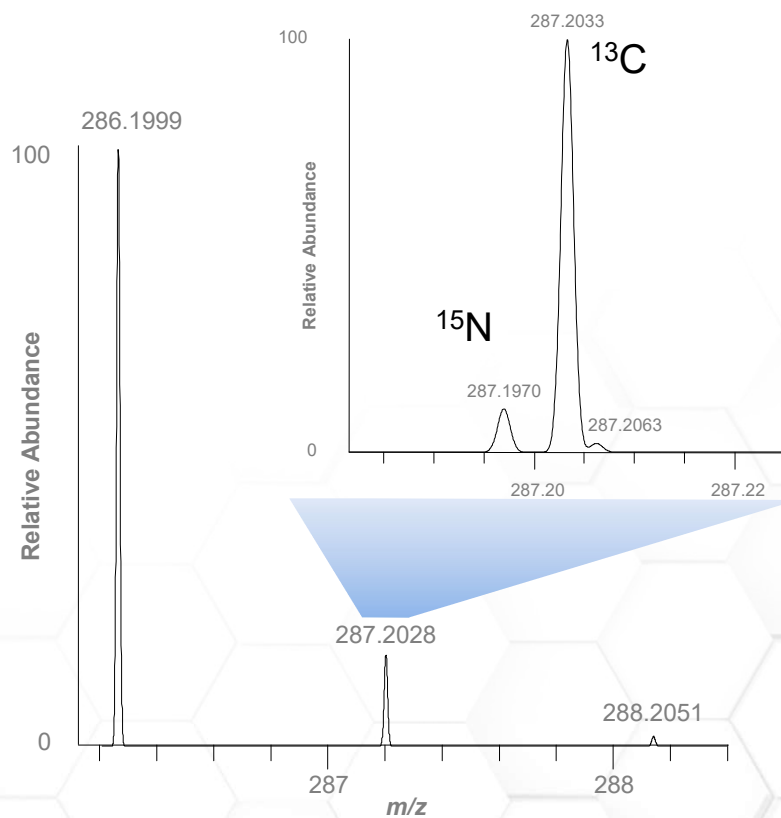




or

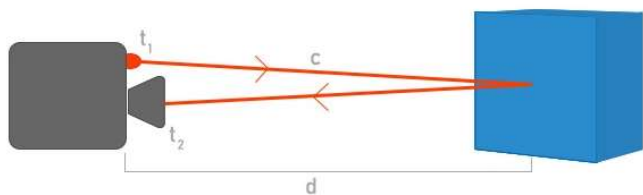


- přesná hmota a popis fragmentů nejsou jediné nástroje
- přesná hmota vede k elementárnímu složení
- velmi vysoké rozlišení značně pomůže ke zpřesnění elementárního složení

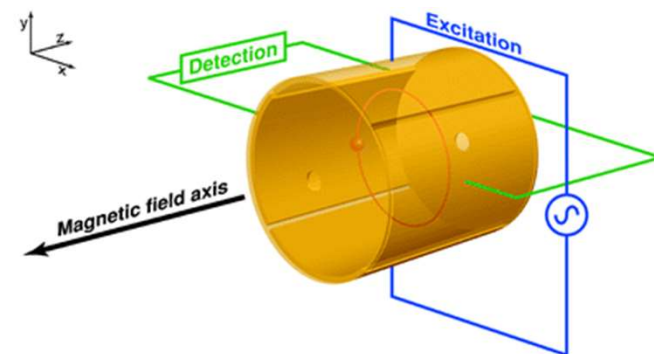


HRAM

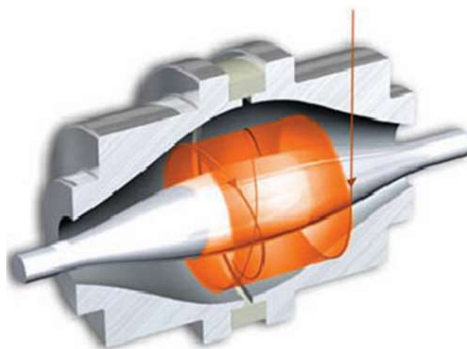
Moderní HRMS



TIME OF FLIGHT (1946)

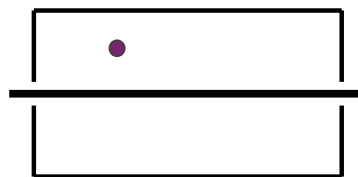


ION CYCLOTRON RESONANCE (1974)

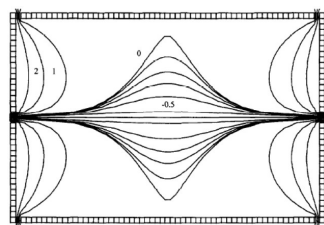


ORBITAL TRAP (2000)

HD Technologies (Hoffman, Davis + Makarov)



Kingdonova past (1923)

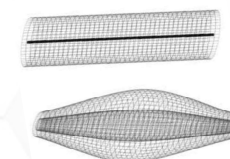


Gillingova past (1996)

1996 HD Technologies

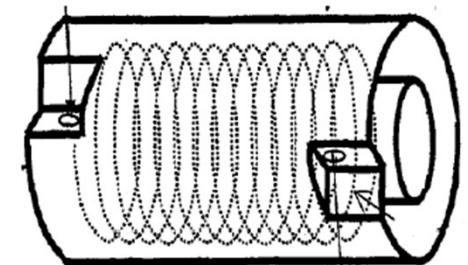
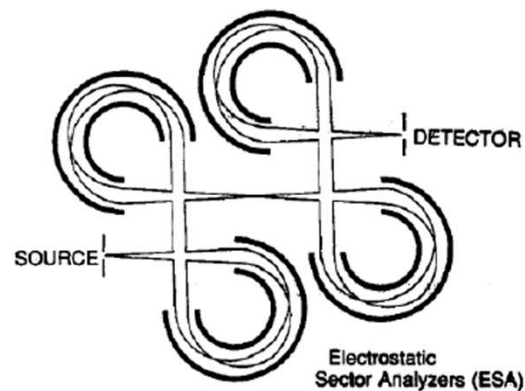
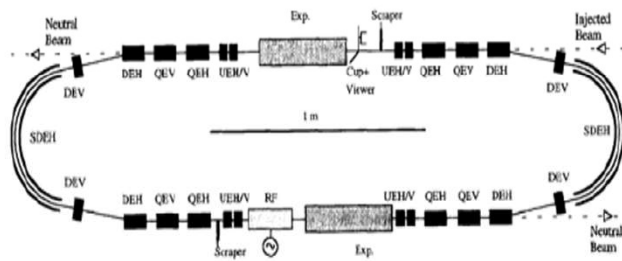
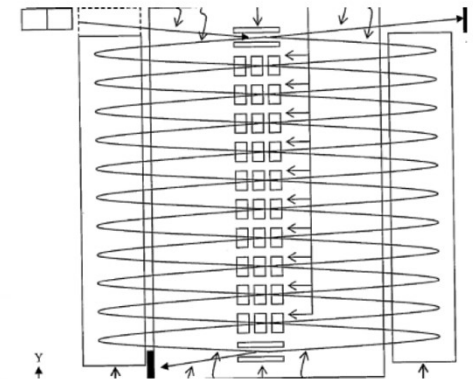
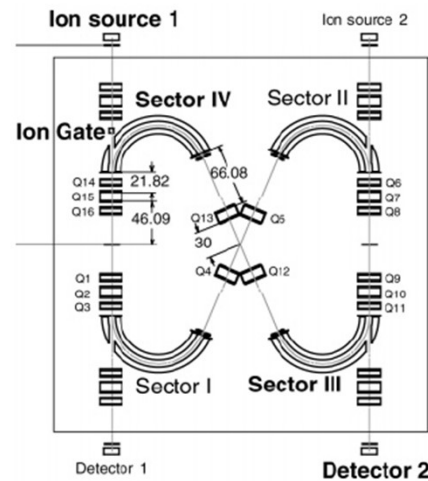
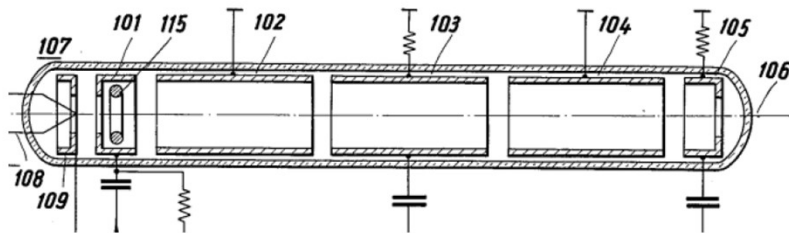
1999 vývoj past'ových
analyzátorů

1999 „Orbitrap“



1999 ASMS, Dallas

Vývoj elektrostatických pastí



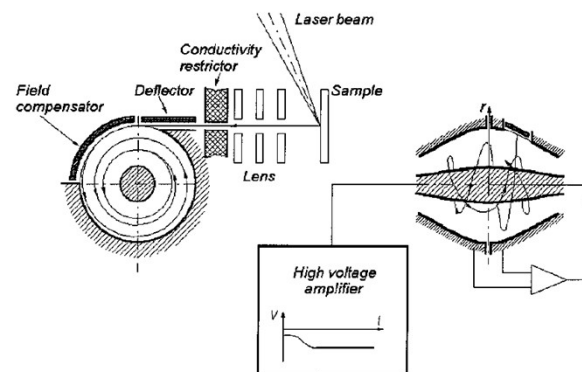
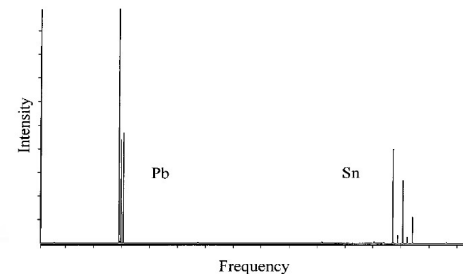
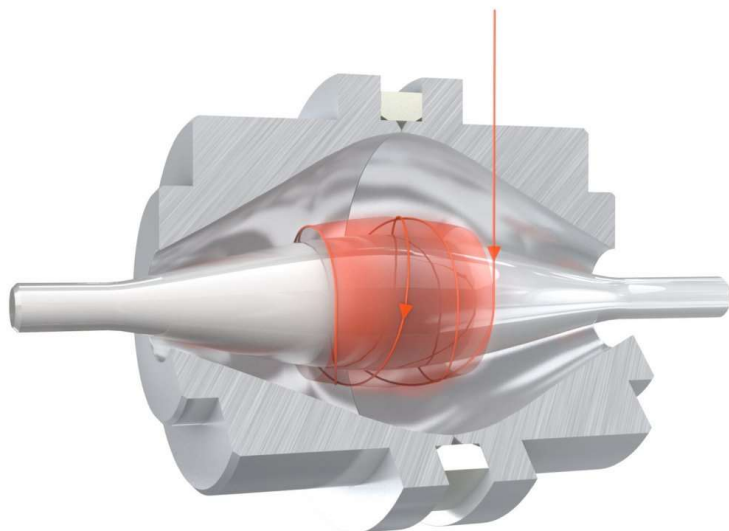
2000 Thermo kupuje HD Technologies

Anal. Chem. 2000, 72, 1156–1162

Electrostatic Axially Harmonic Orbital Trapping: A High-Performance Technique of Mass Analysis

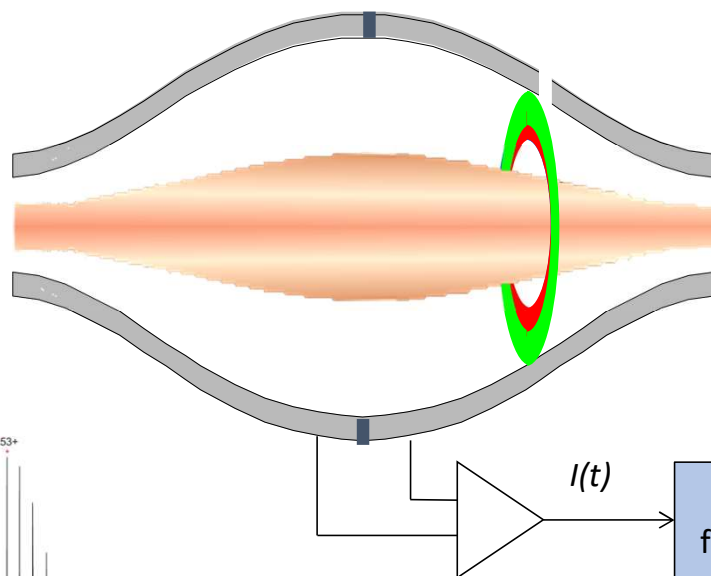
Alexander Makarov*

HD Technologies Ltd., Atlas House, Simonsway, Manchester, M22 5PP, U.K.



pragolab

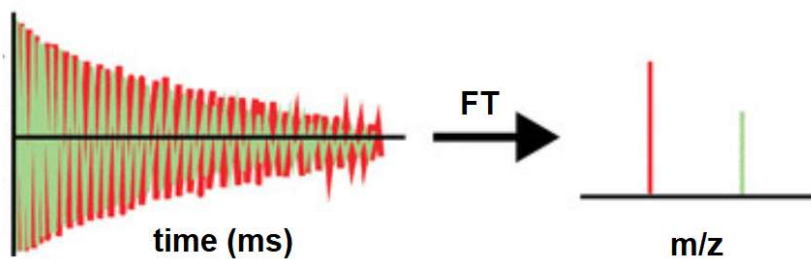
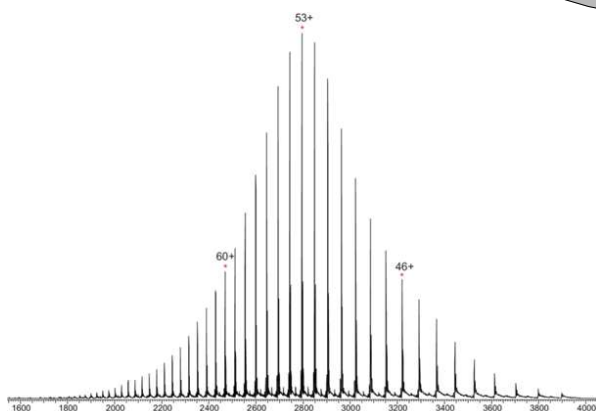
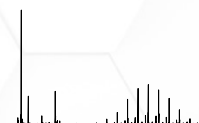
pojem „skenování“ prosím s rezervou



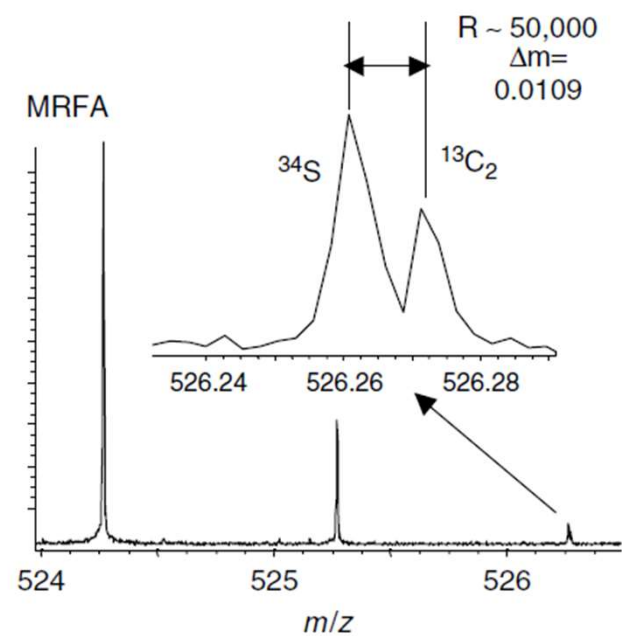
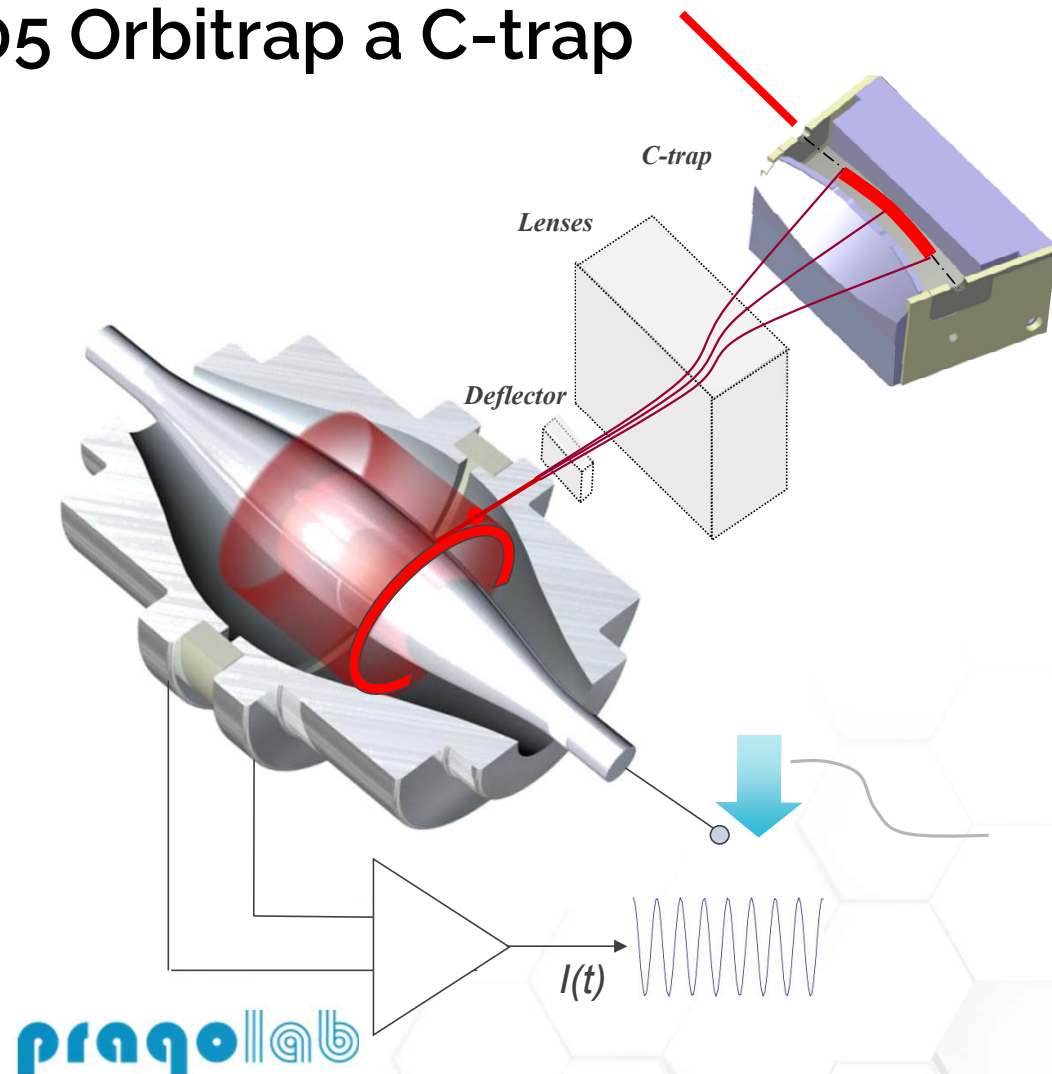
$$F(\omega_m) = \sum_{n=0}^{N-1} f(t_n) \exp\left(\frac{-inm}{N}\right)$$

+ zero filling
+ apodization
....

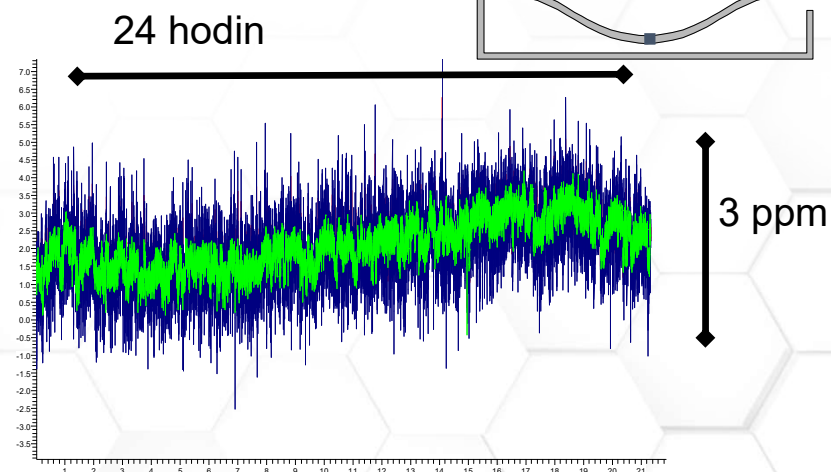
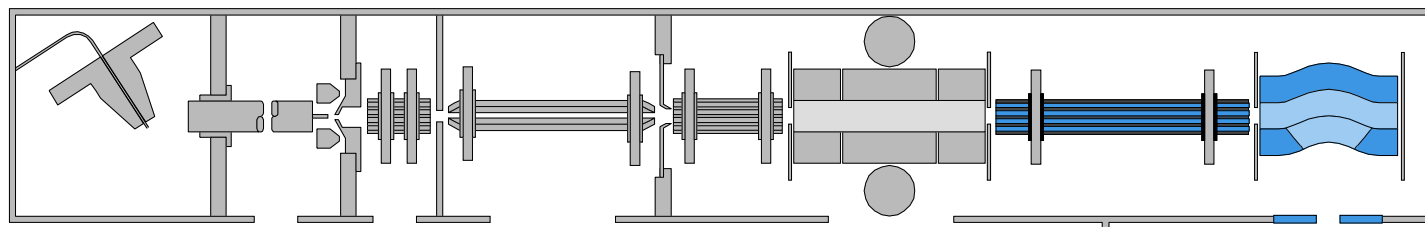
int(m/z)



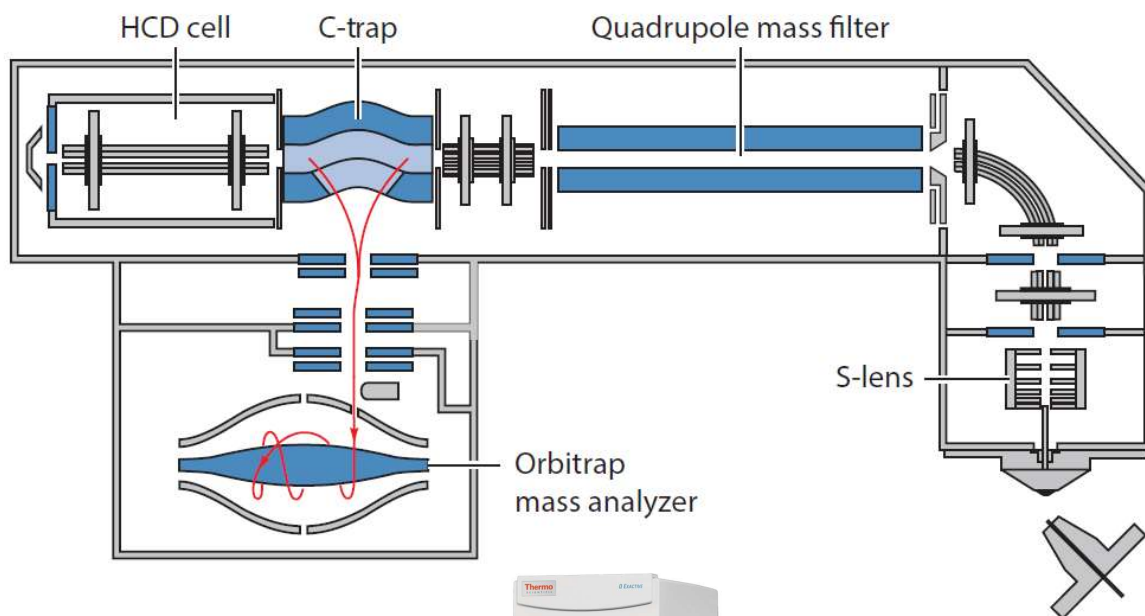
2005 Orbitrap a C-trap



2005 LTQ Orbitrap

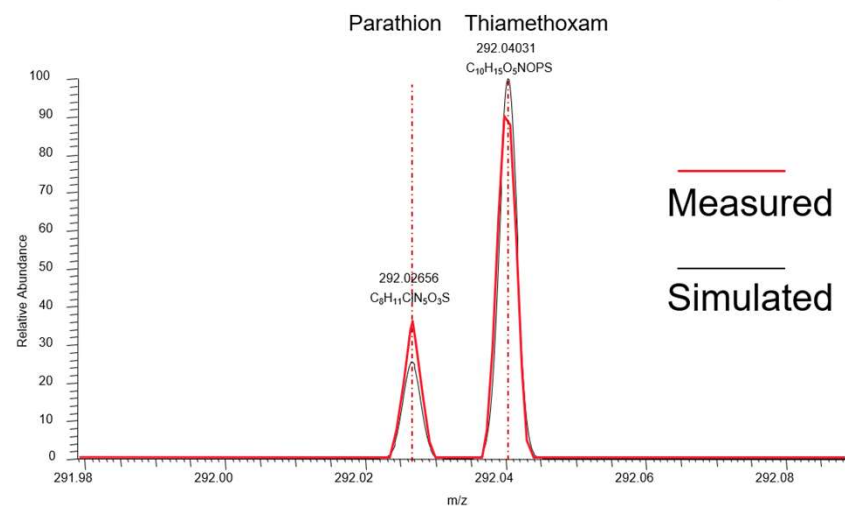


2008-2011 Exactive a Q Exactive



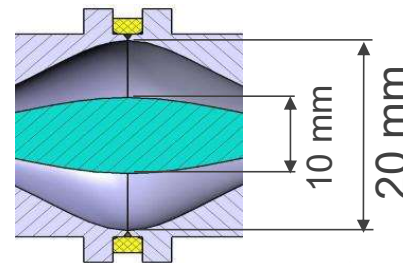
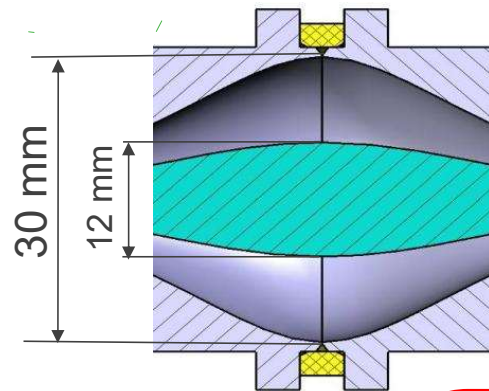
pragolab

$R = 100\,000$

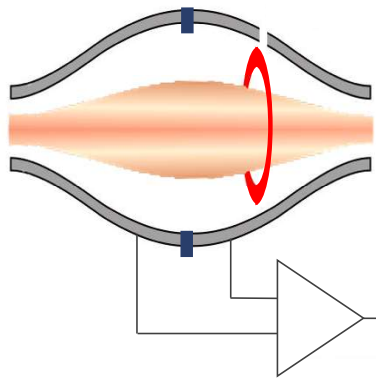




2011 High Field Orbitrap + eFT = 4x vyšší rozlišení



HIGH FIELD ORBITRAP



pragolab

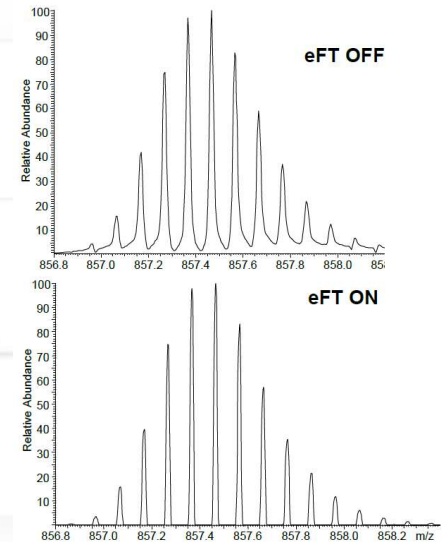
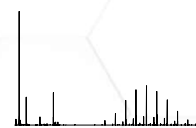
$$F(\omega_m) = \sum_{n=0}^{N-1} f(t_n) \exp\left(\frac{-inm}{N}\right)$$

+ zero filling
+ apodization

....

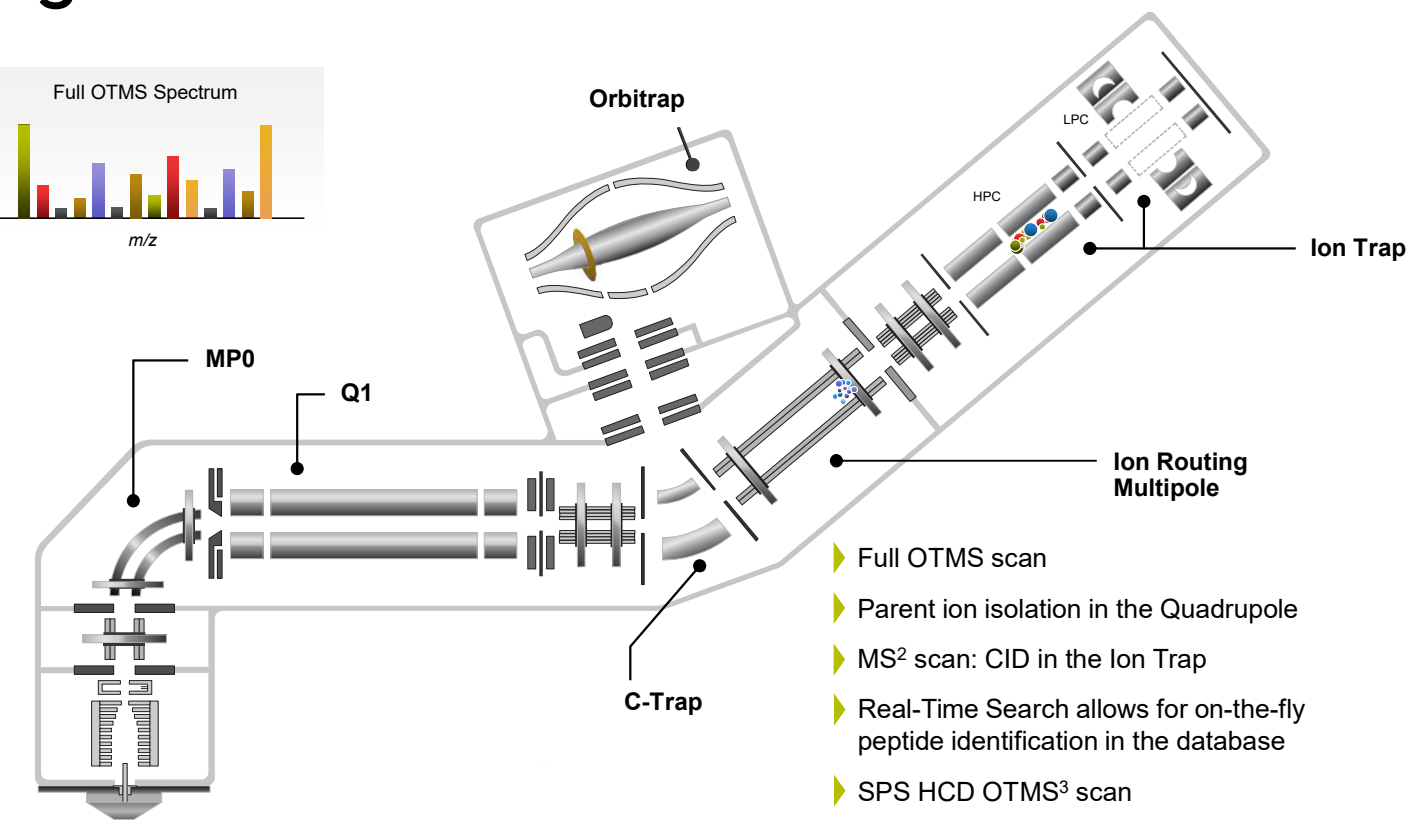
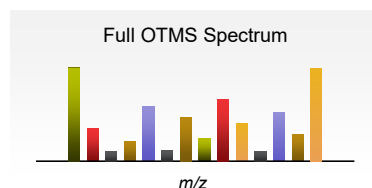
FFT +
processing

$int(m/z)$

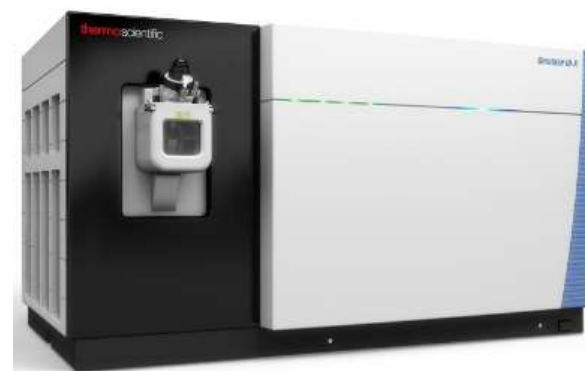




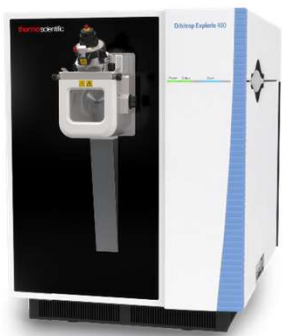
2013 tribrides



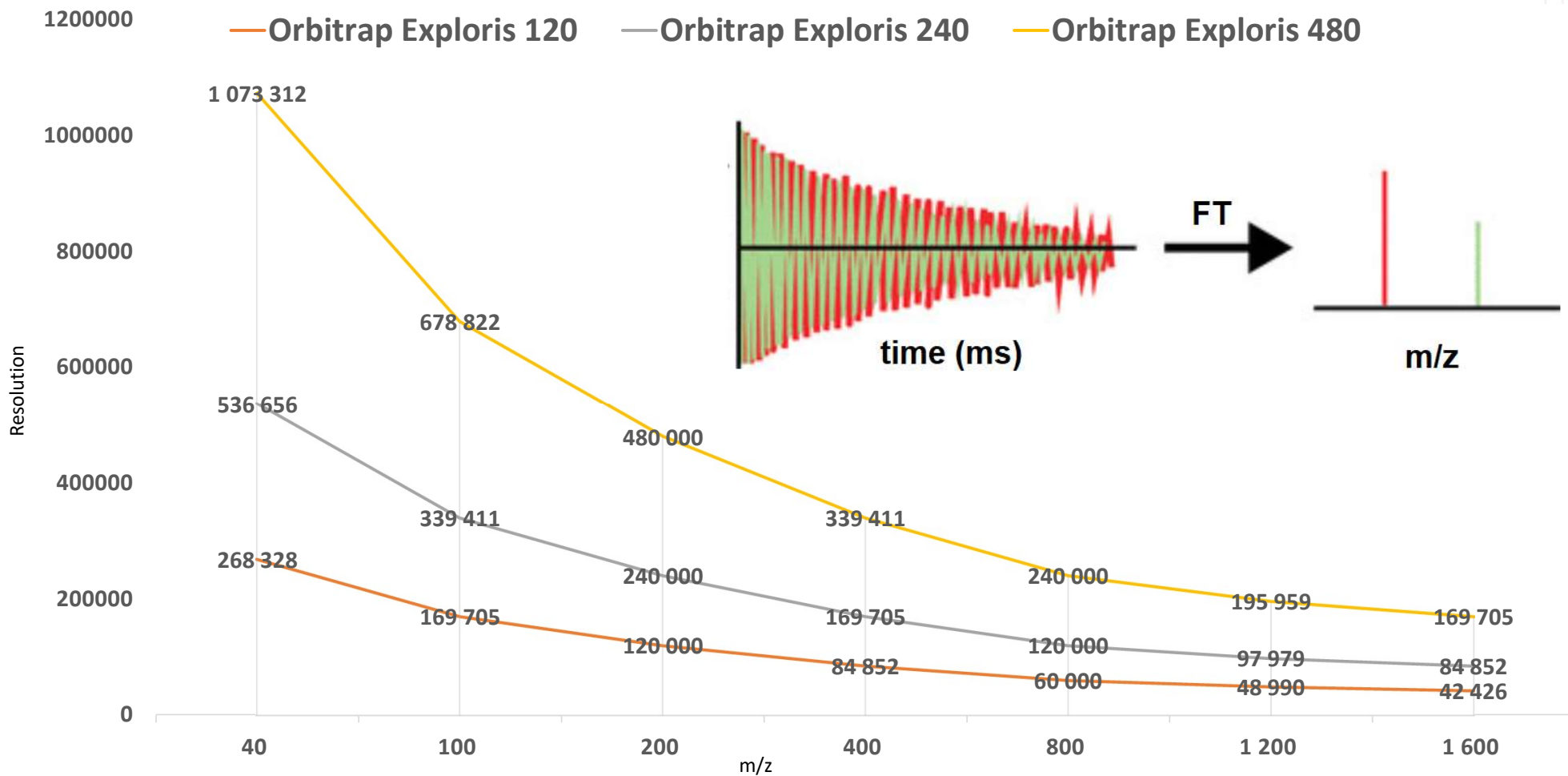
- ▶ Full OTMS scan
- ▶ Parent ion isolation in the Quadrupole
- ▶ MS² scan: CID in the Ion Trap
- ▶ Real-Time Search allows for on-the-fly peptide identification in the database
- ▶ SPS HCD OTMS³ scan
 - Synchronous Precursor Selection of only the b fragments in the Ion Trap
 - HCD MS³
 - OTMS detection of MS³ fragments

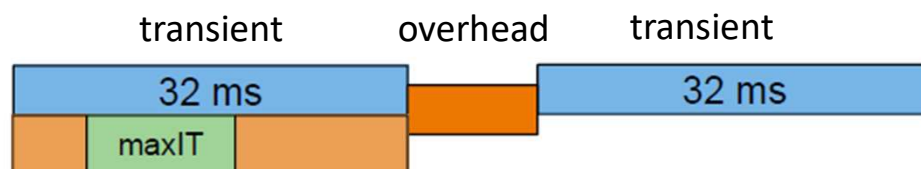


2019

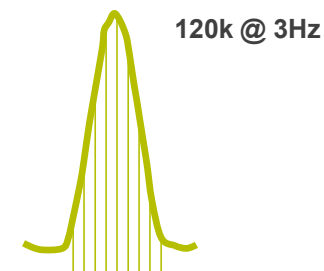


pragolab

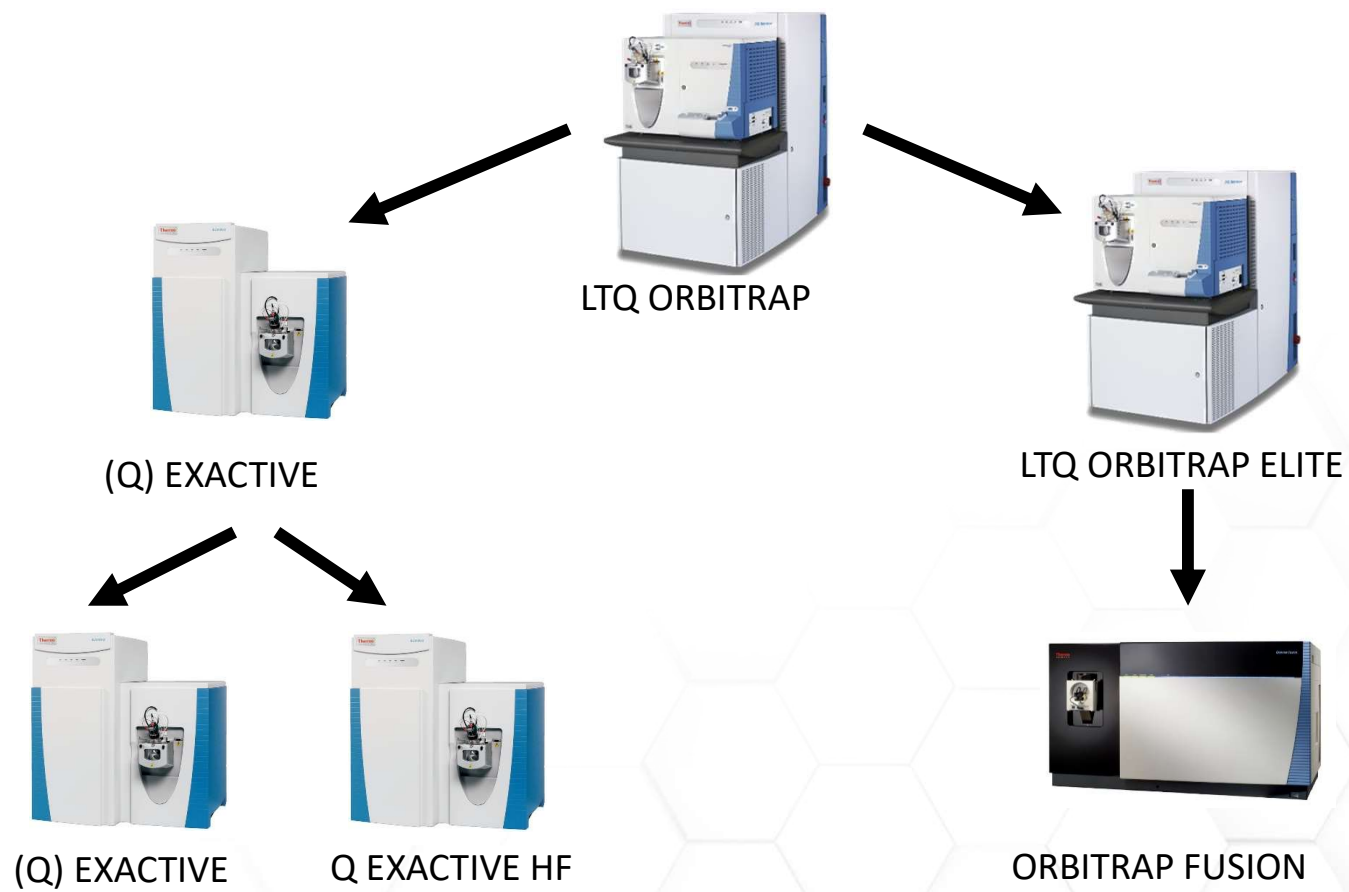




rozlišení	transient	vzorkování
7 500	16 ms	40 Hz
15 000	32 ms	22 Hz
30 000	64 ms	12 Hz
60 000	128 ms	7 Hz
120 000	256 ms	3 Hz
240 000	512 ms	2 Hz
480 000	1024 ms	1 Hz



Points Across the Peak 9



2022



(Q) EXACTIVE



Q EXACTIVE HF



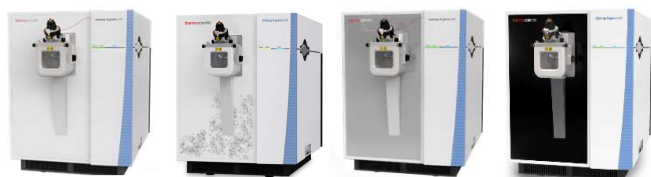
ORBITRAP FUSION



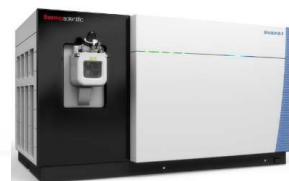
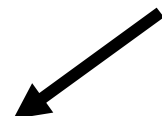
QE FOCUS
QE PLUS



QE HF-X



EXPLORIS
(120/MX/240/480)



ID-X, IQ-X

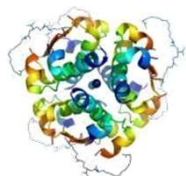


LUMOS



ECLIPSE



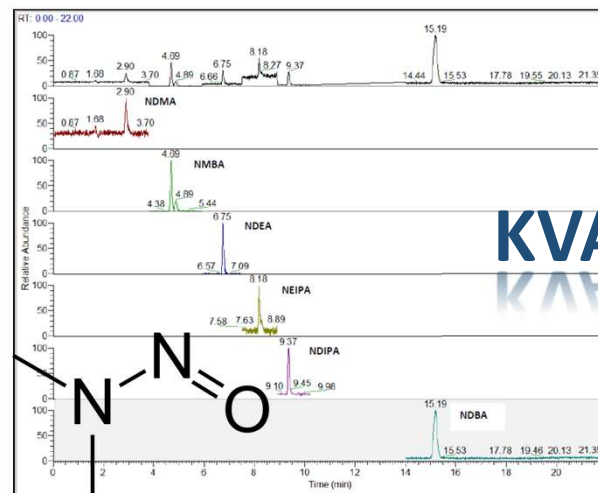


BIOPHARMA

KVANTITA

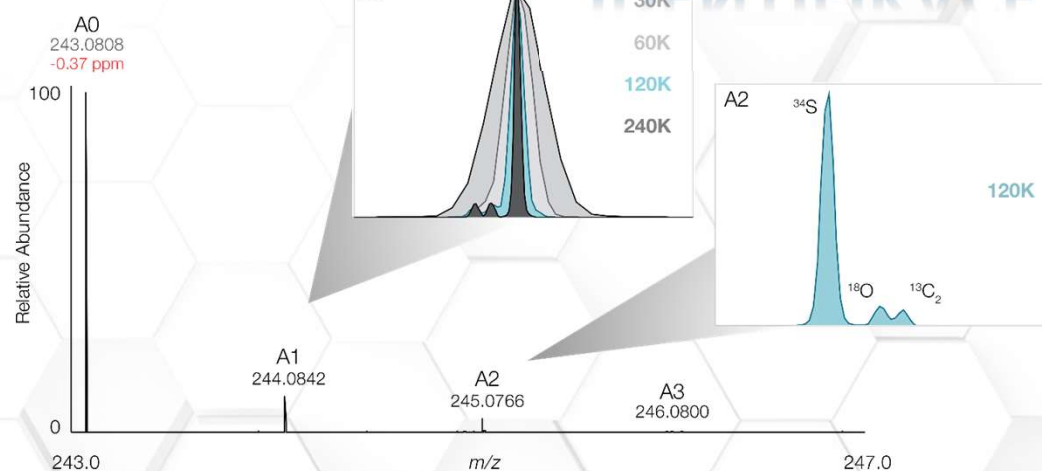
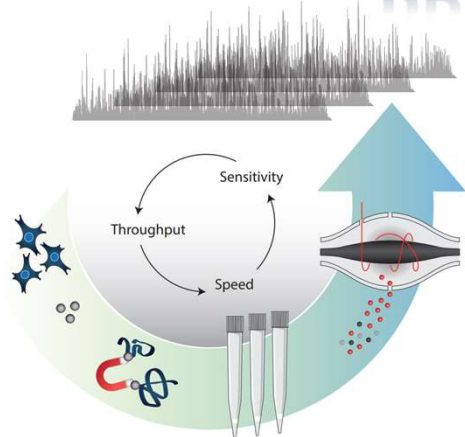
Combined

NDMA
(EIC m/z
75.0553)
NMBA
(EIC m/z
145.0619)
NDEA
(EIC of m/z
75.0553,
103.0866)
NEIPA
(EIC m/z
75.0553)
NDIPA
(EIC m/z
131.1179)
NDBA
(EIC m/z
57.0704,
103.0872,
159.1492)



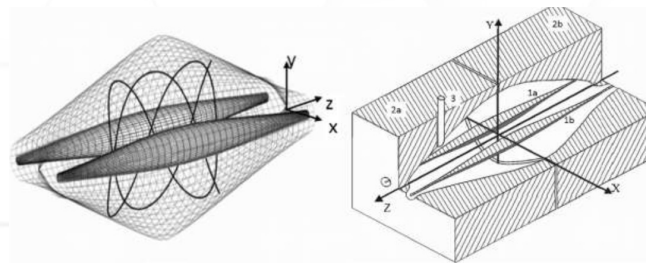
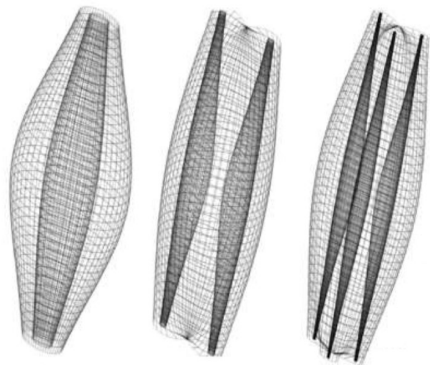
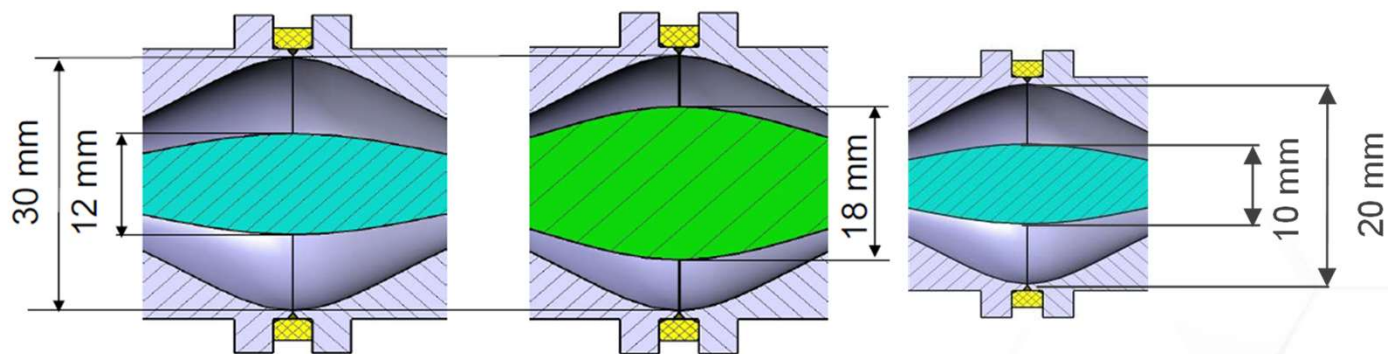
PROTEOMIKA

IDENTIFIKACE



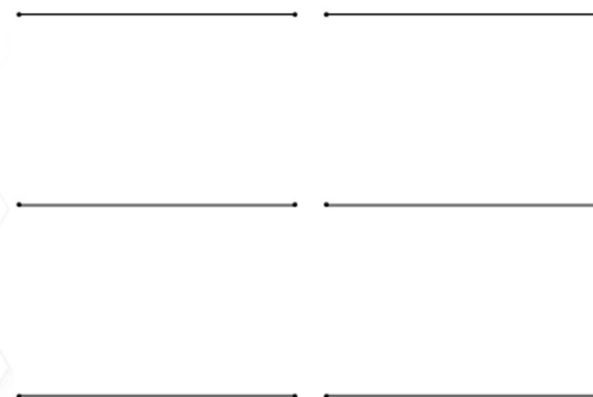
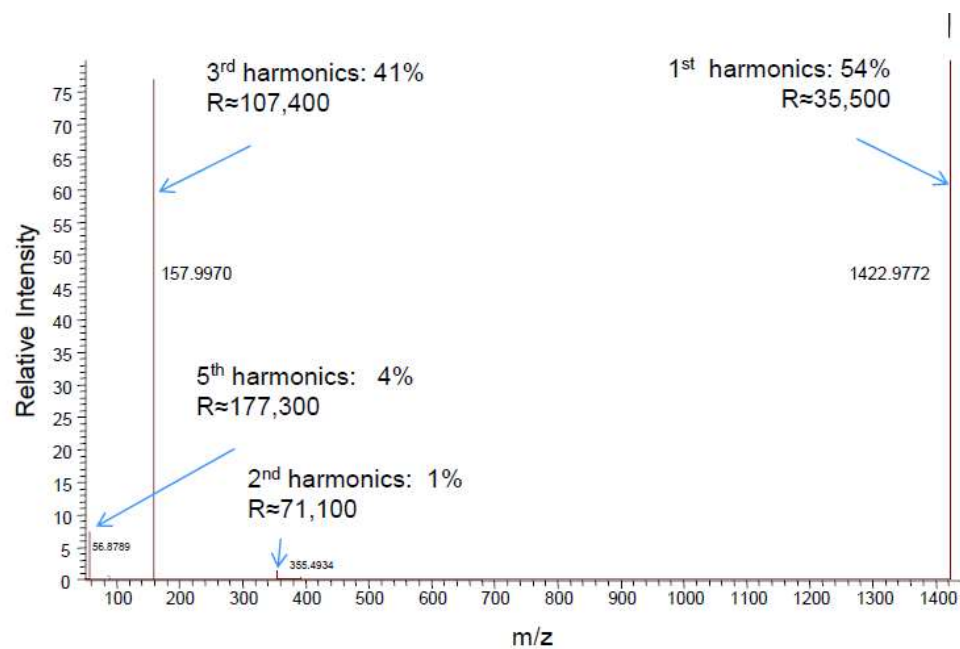
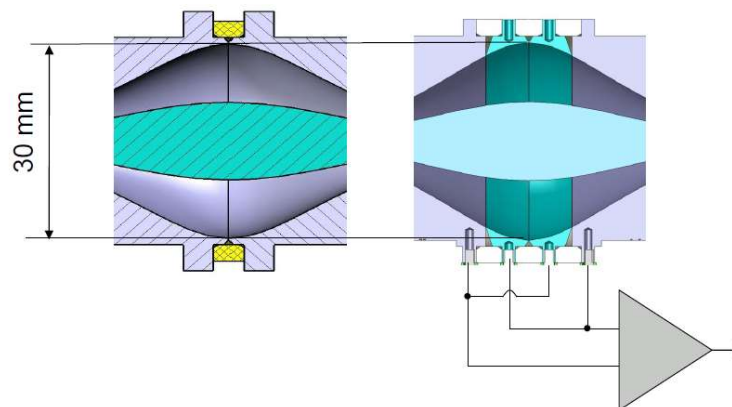
2022 – prostor k rozvoji?

1. NOVÉ GEOMETRIE



2022-dále

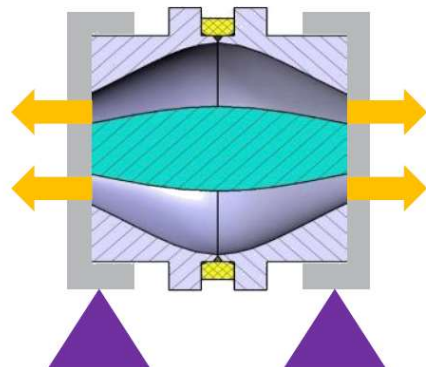
2. VYŠŠÍ HARMONICKÉ



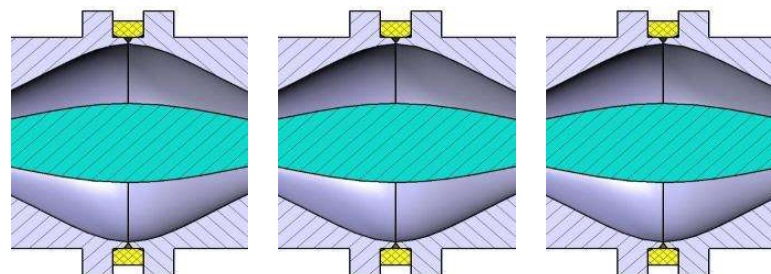
2022-dále

3. VYLEPŠENÍ

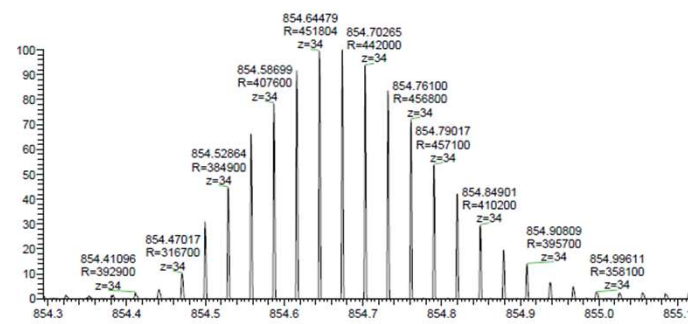
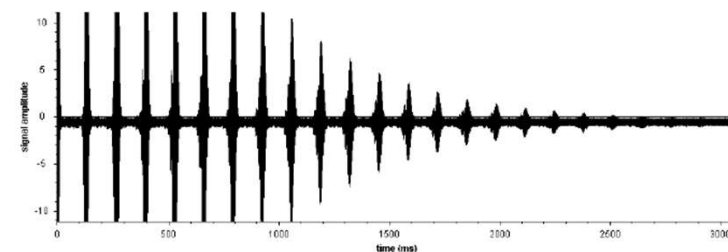
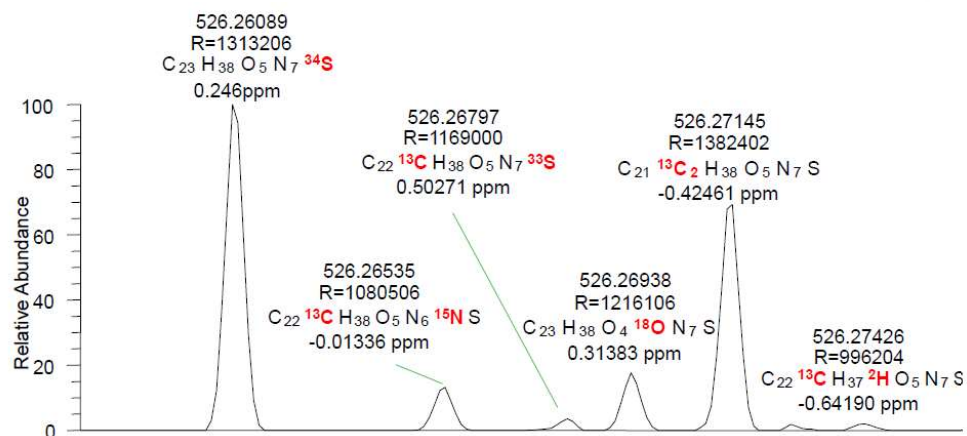
Streamlined ultra-precise electrodes



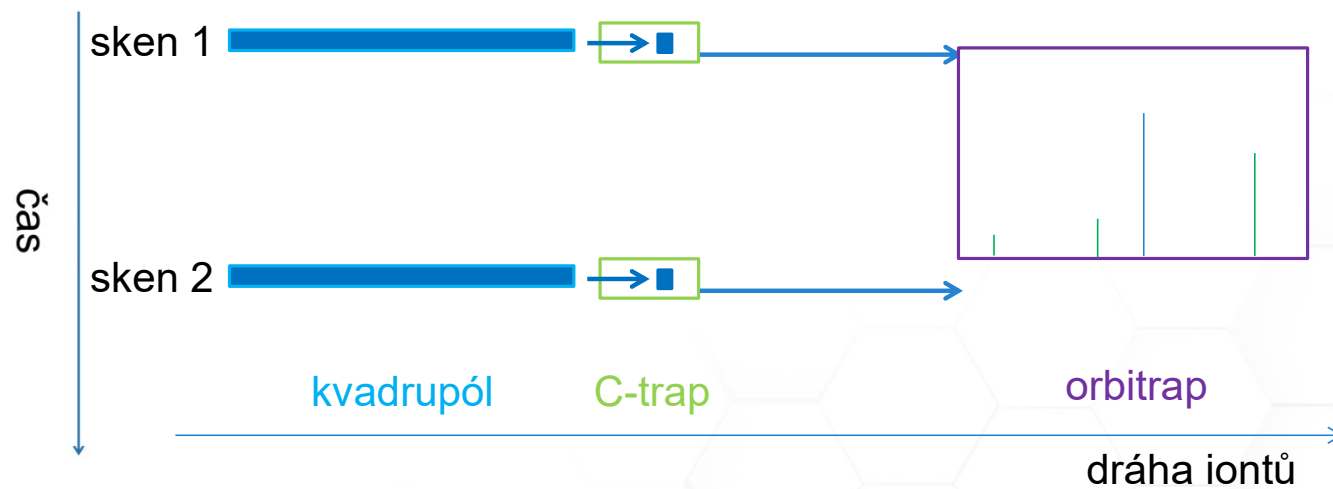
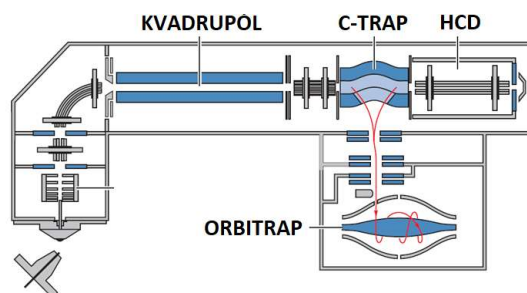
Improved pumping



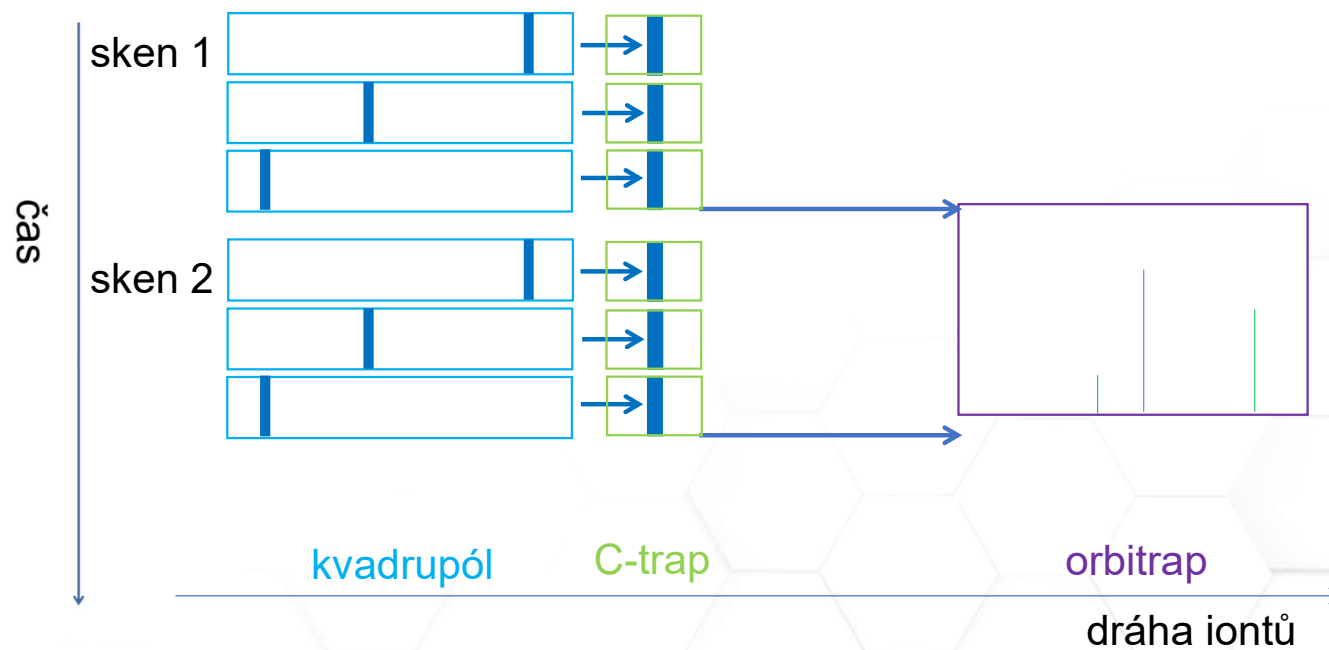
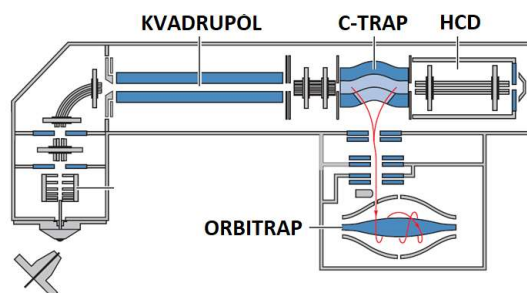
Symmetrical mechanical support



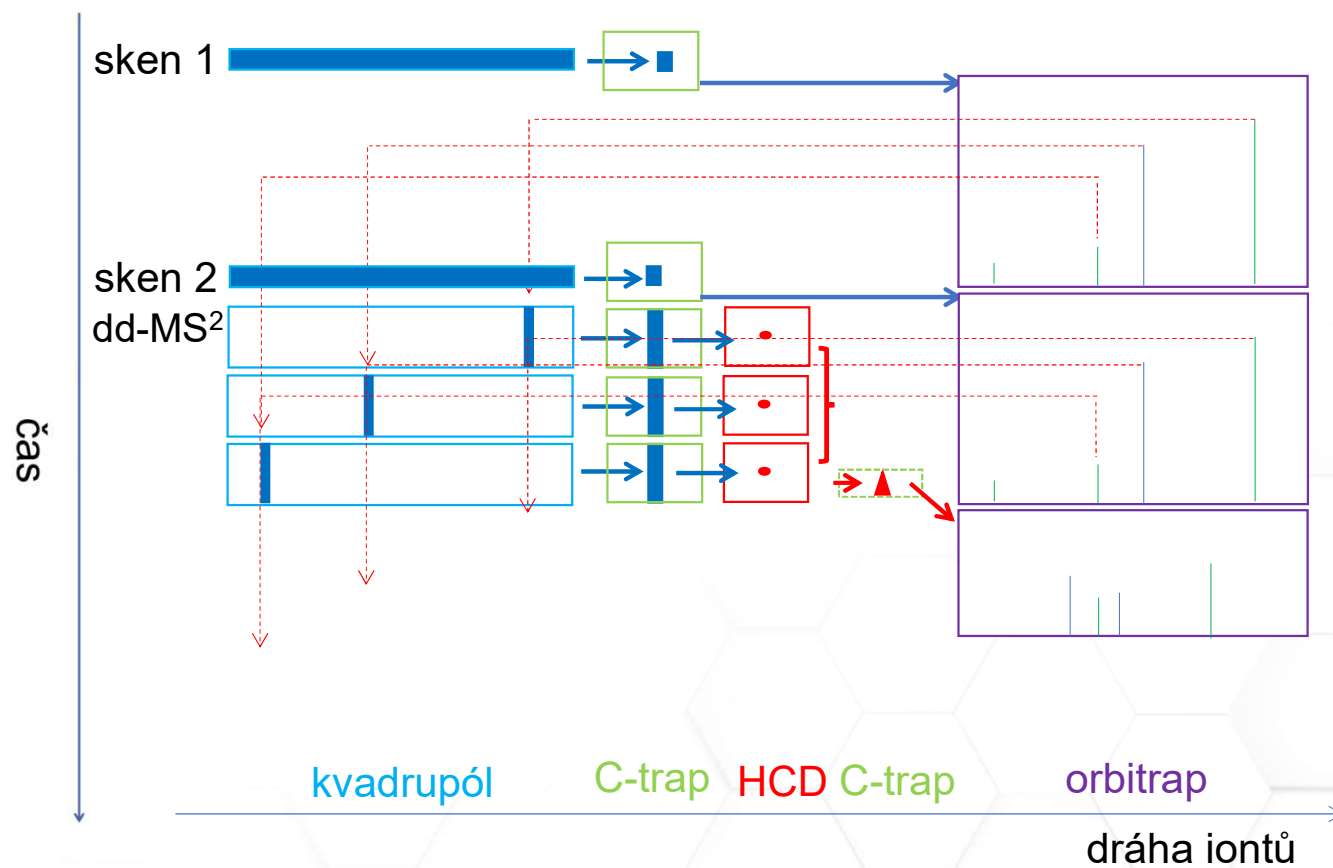
2022-dále



2022-dále



2022-dále





praqollab