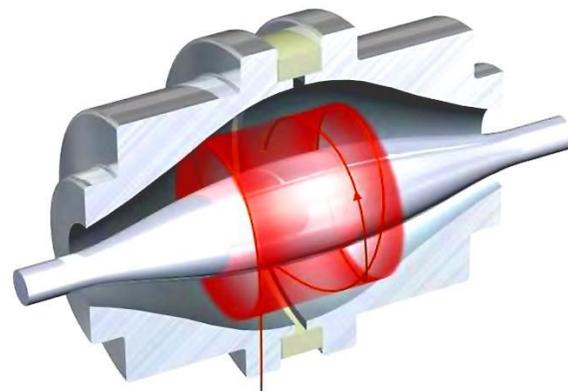


pragolab

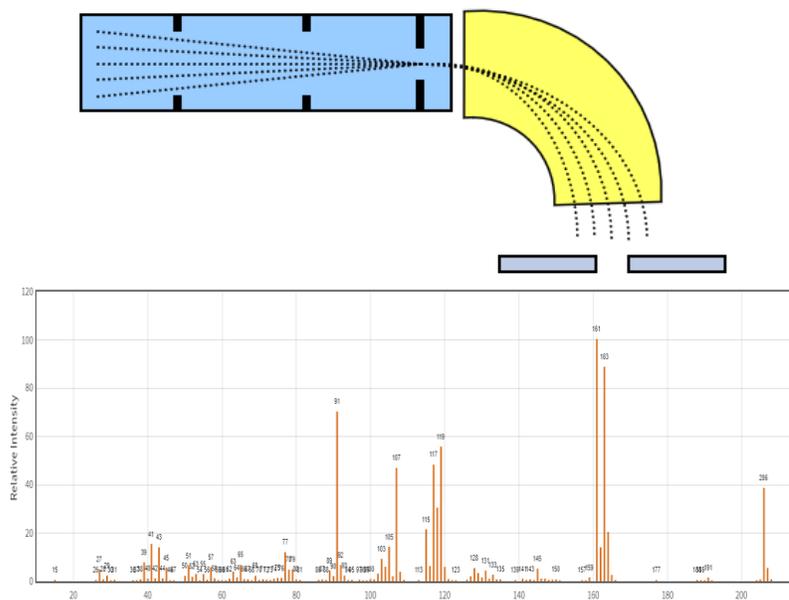
# „Hvězdné“ hybridní spektrometry



Lukáš Plaček  
&  
Roman Hájek

# Vývojová etapa 1

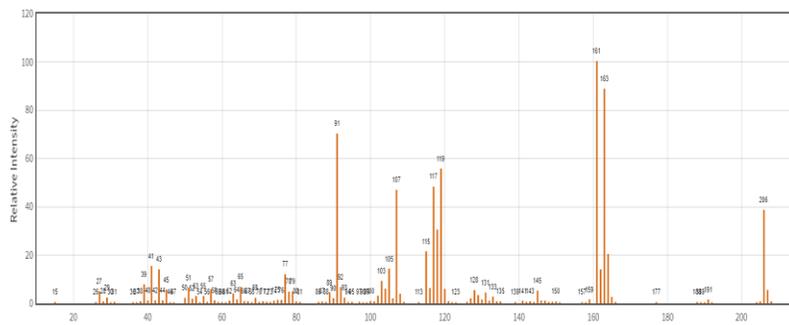
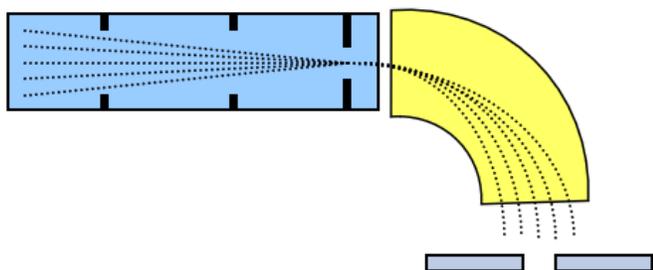
# MS



studium dějů  
v plynné fázi

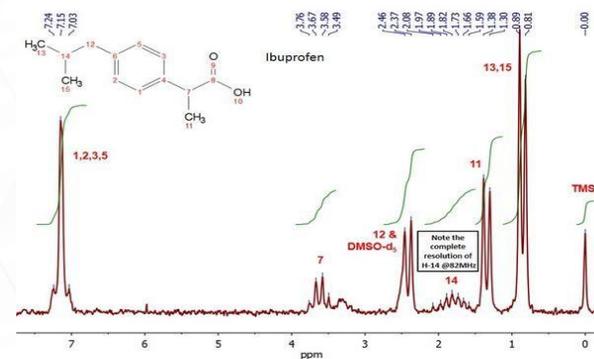
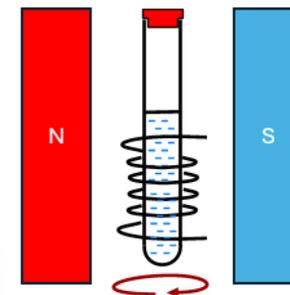
# Vývojová etapa 2

# MS



+

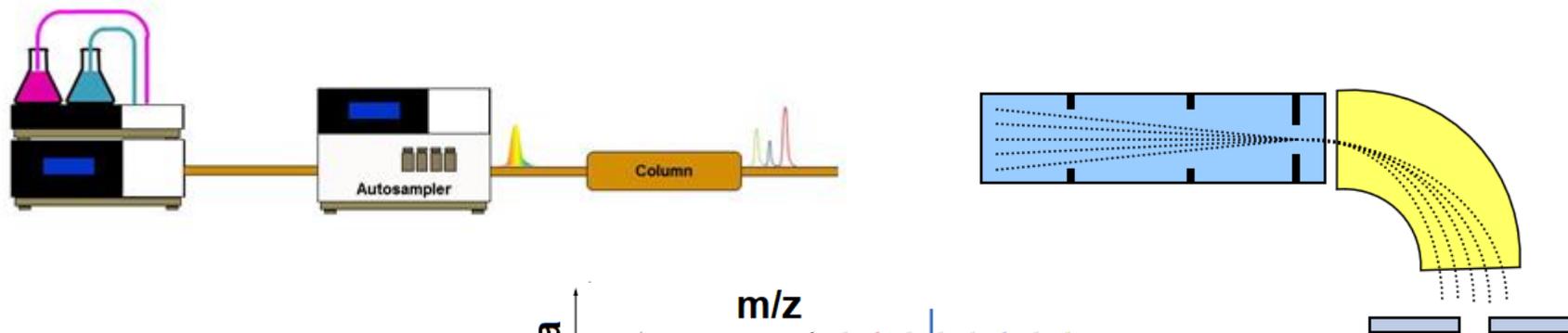
# NMR



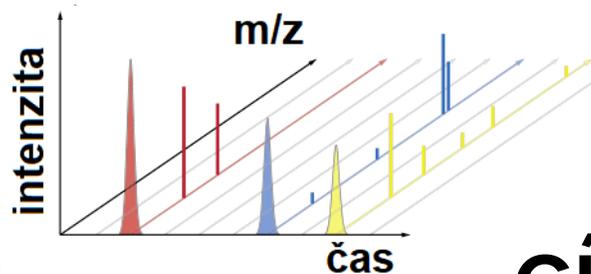
# strukturní analýza

# Vývojová etapa 3

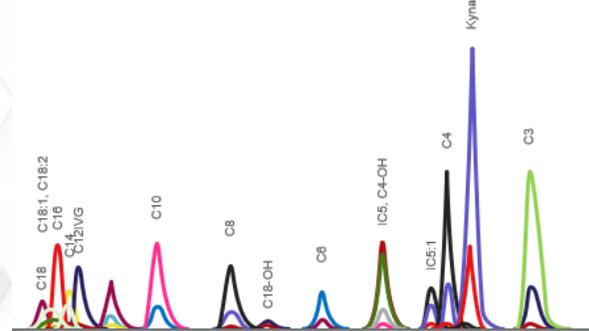
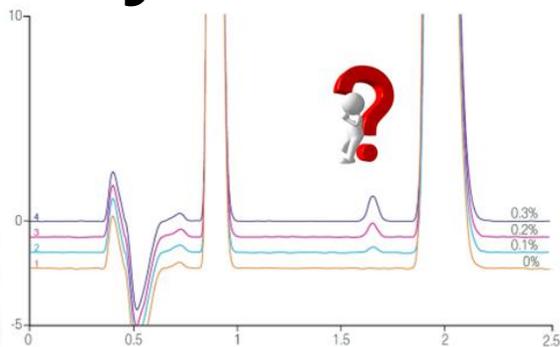
# xC-MS



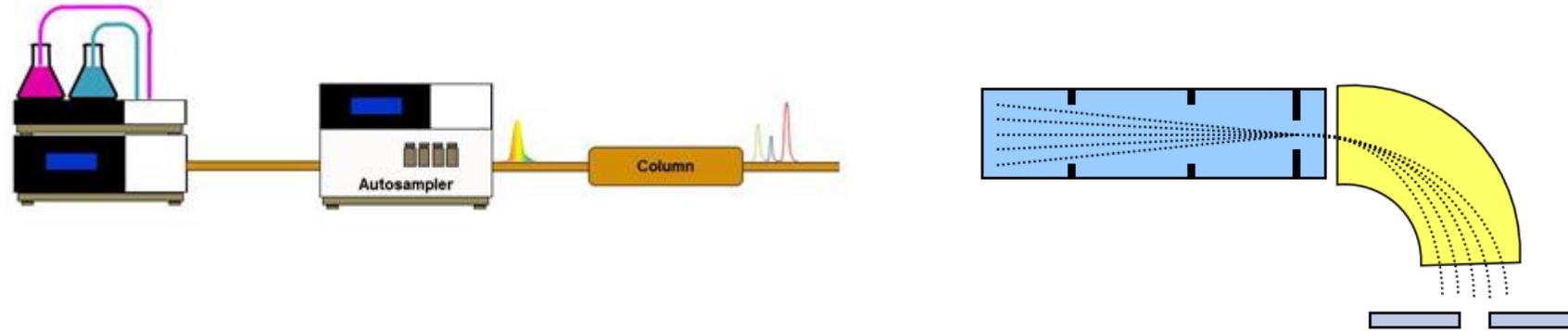
**strukturní analýza  
analytů ve směsi**



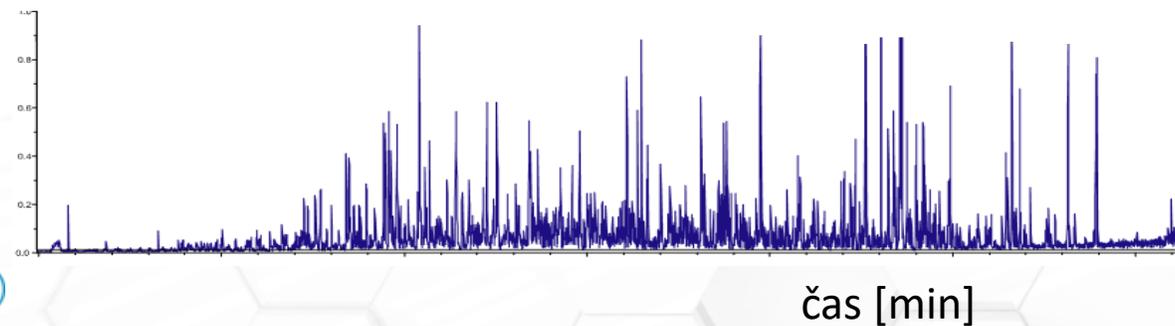
**cílená analýza  
(kvantitativní)**



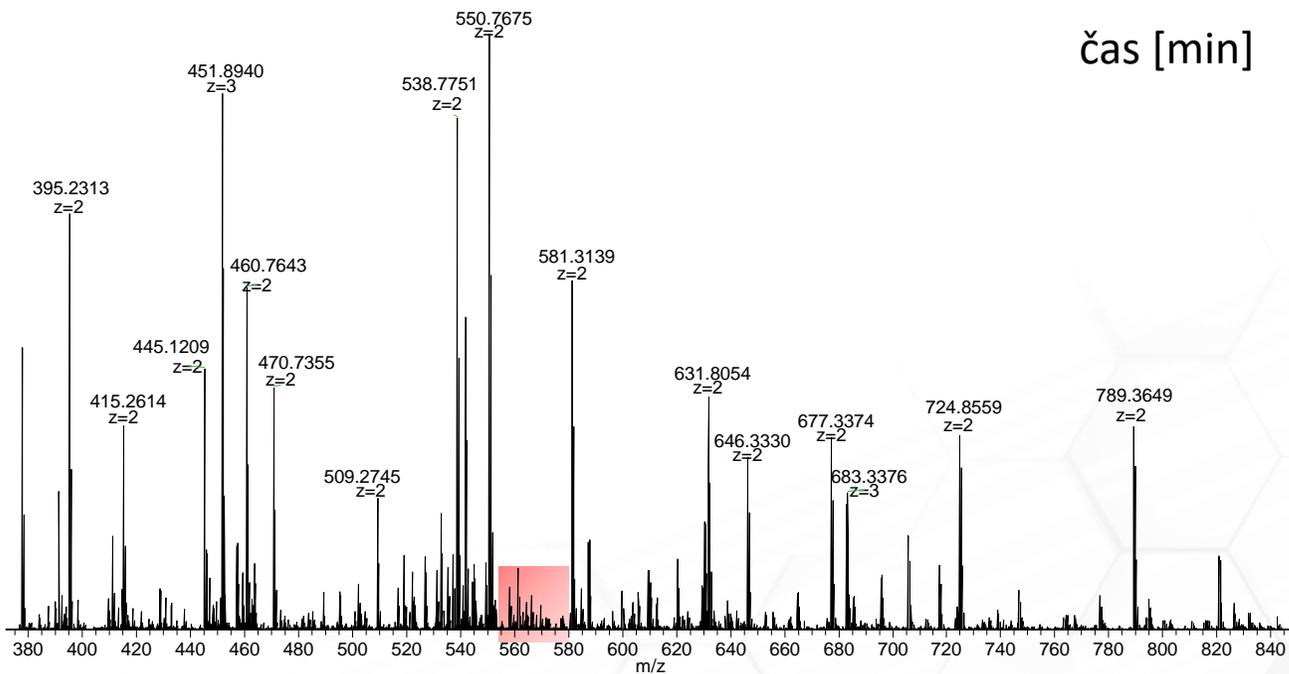
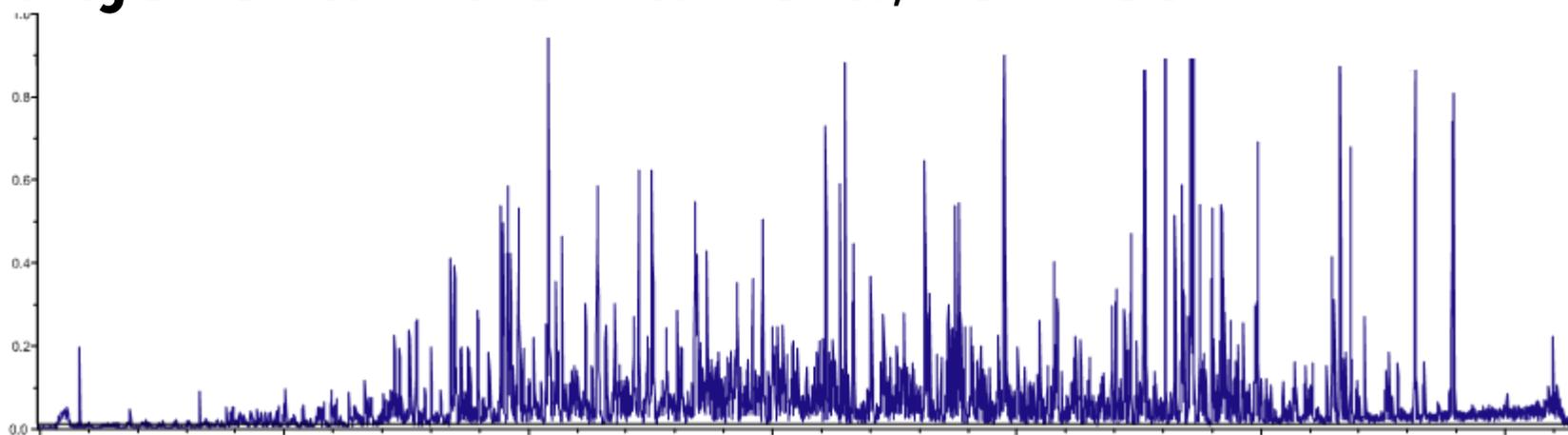
# xC-MS



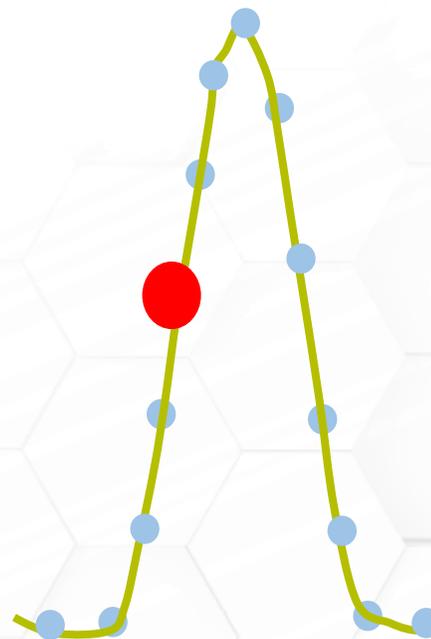
**necílená analýza  
(strukturní + semikvantitativní)**



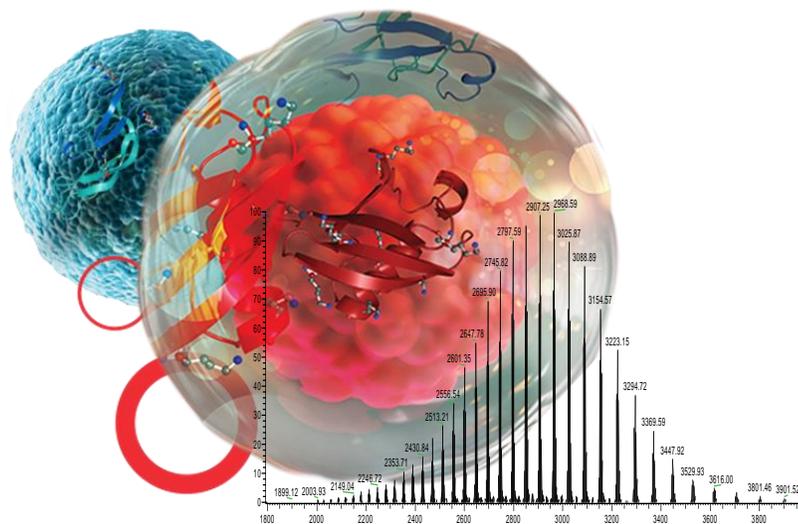
# Objevování biomarkerů, -omics



čas [min]



# Hmotnostní spektrometrie v moderní léčbě



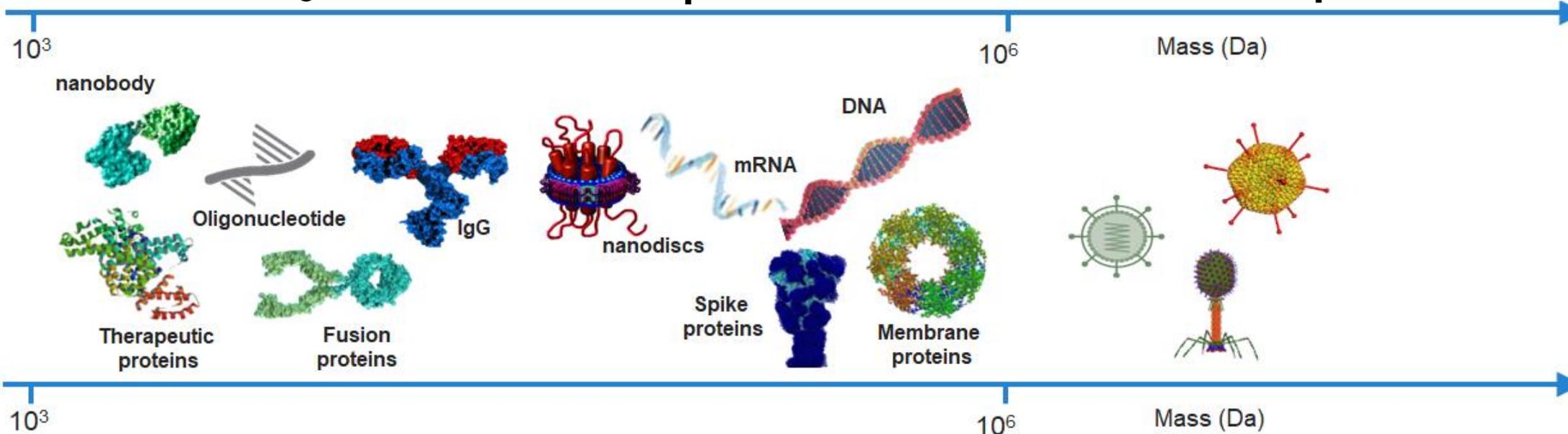
objev



produkce



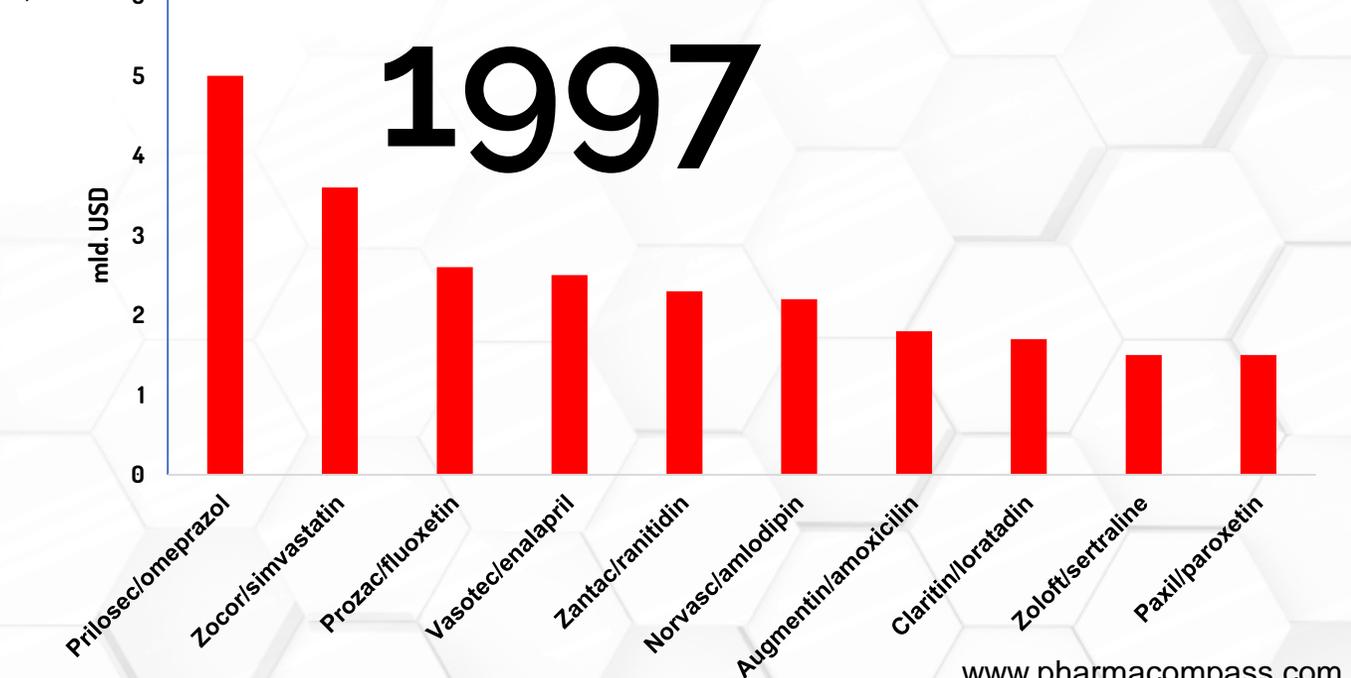
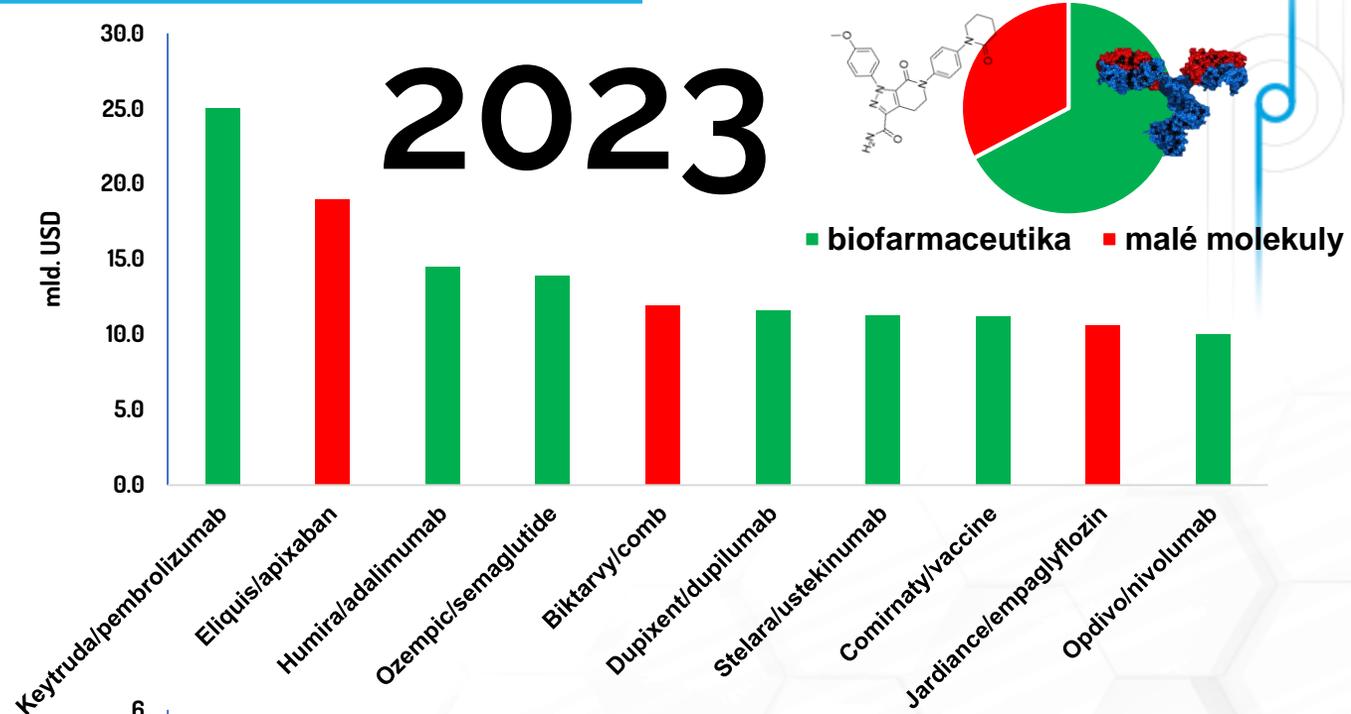
použití



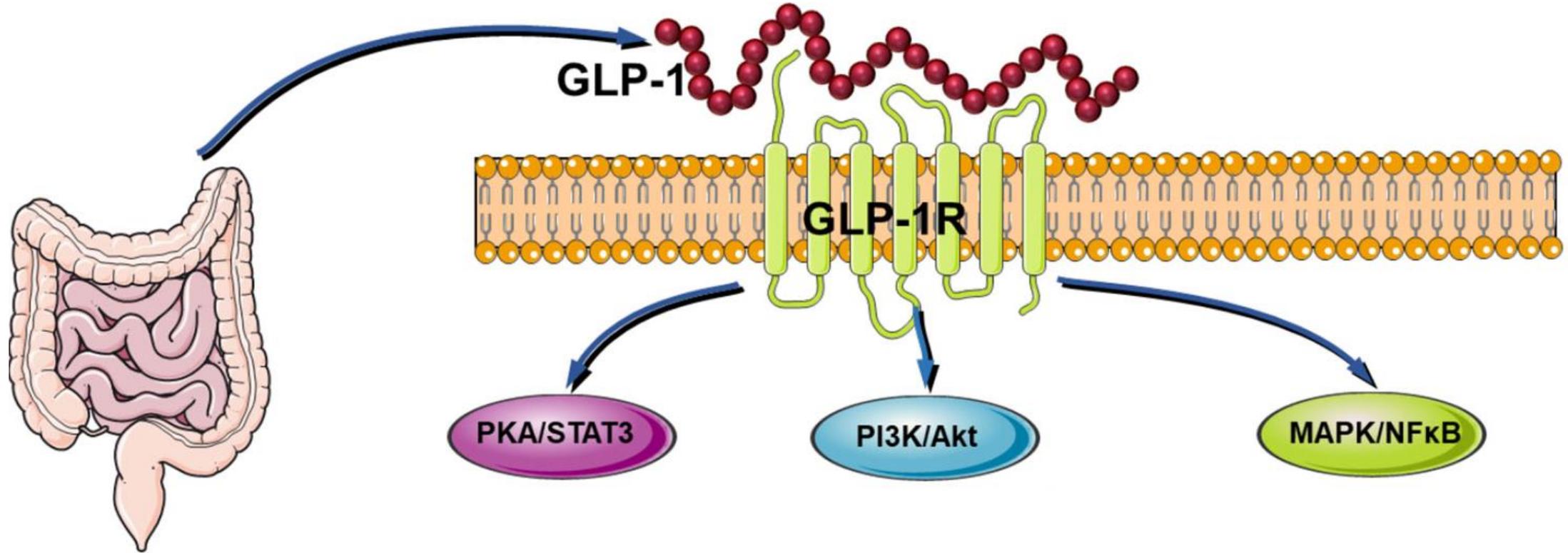
# Tlak na rozvoj hmotnostných spektrometrů



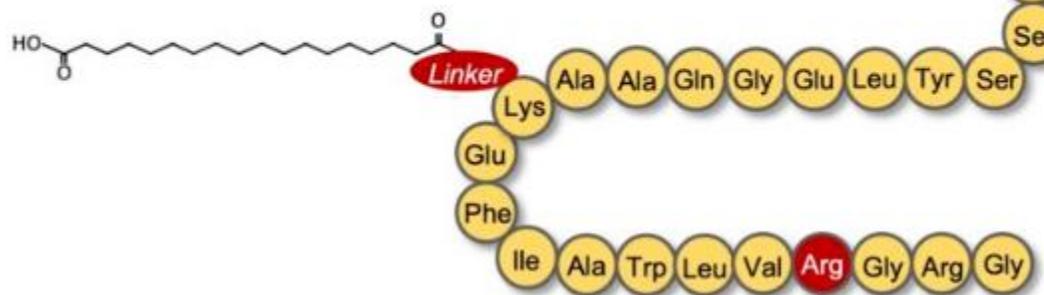
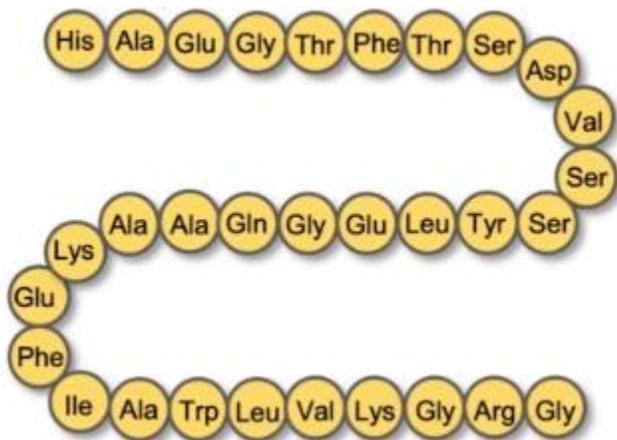
# Trendy moderní léčby



# Ozempic - semaglutid



# Ozempic - semaglutid



## HOSPODÁŘSKÉ NOVINY

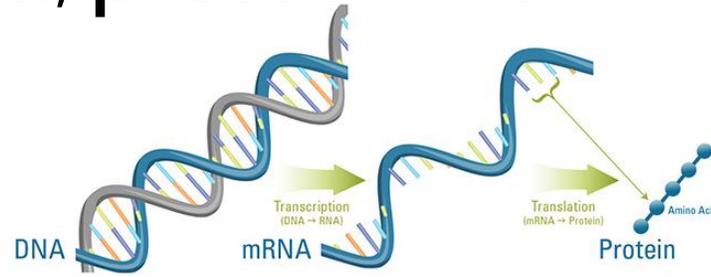
Hledat

BYZNYS ZPRÁVY NÁZORY TECH REALITY INVESTICE PODCASTY PročNe ARCHIV DALŠÍ

**Největší evropská firma míří do Česka. Chce koupit závod, který teď vyrábí vakcíny proti covidu**



# Genomika, transkriptomika, proteomika



... GTGCATCTGACTCCTGAGGAGAAG ...  
... CACGTAGACTGAGGACTCCTCTTC ...

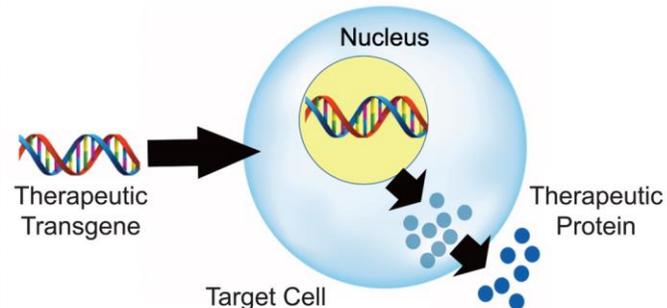
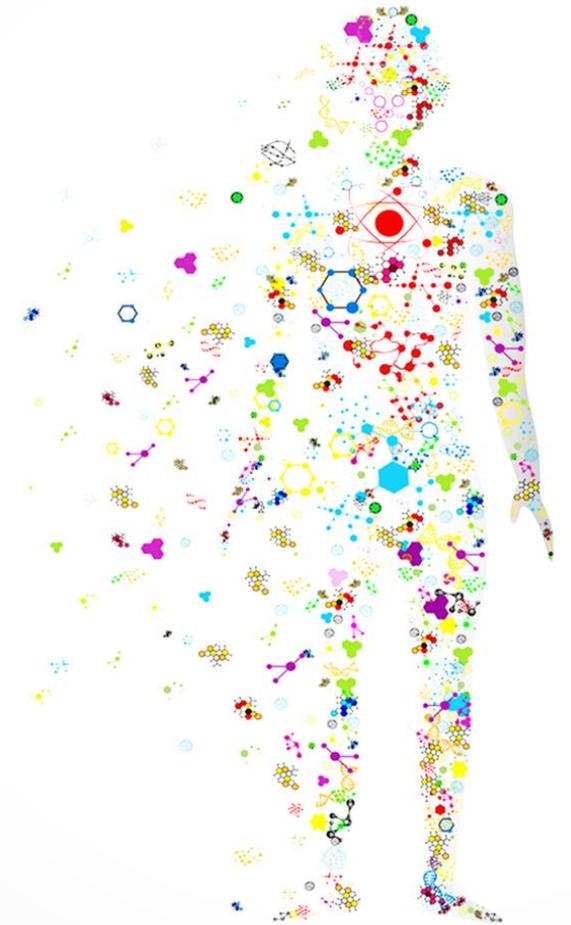
DNA  
(transcription)

... GUGCAUCUGACUCCUGAGGAGAAG ...

RNA  
(translation)

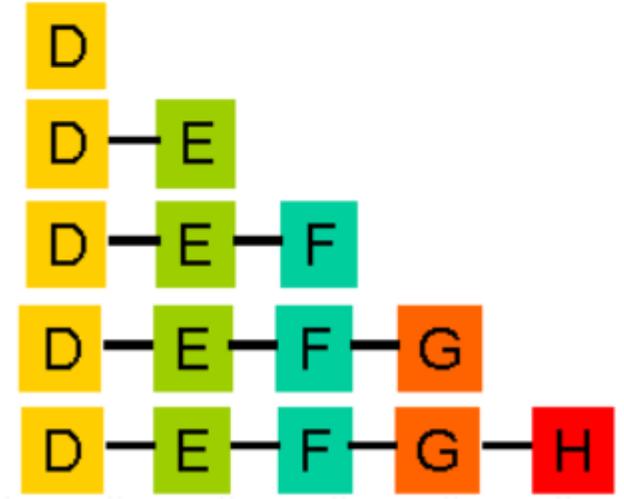
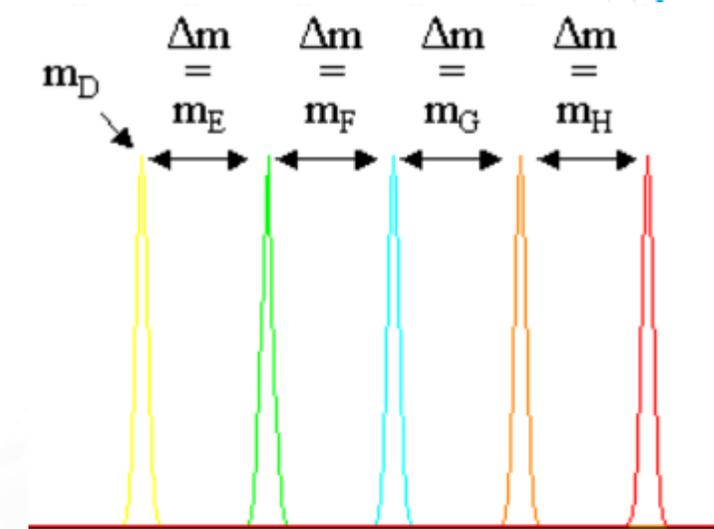
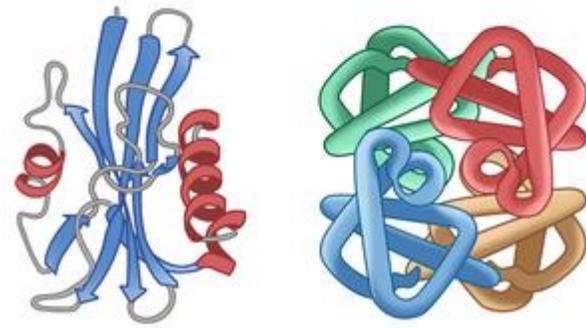
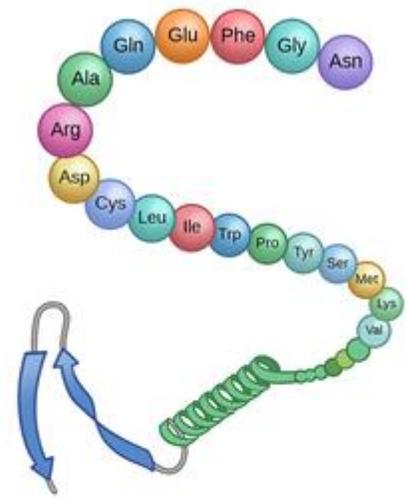
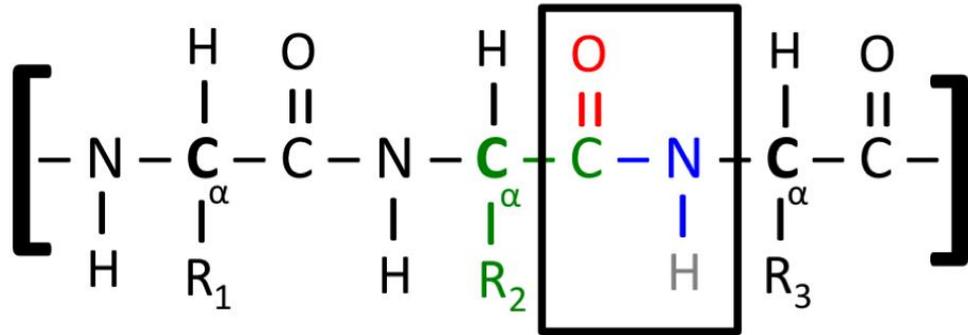
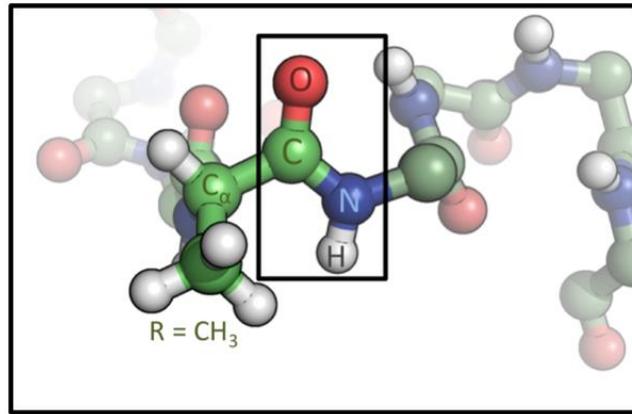
... V-H-L-T-P-E-E-K ...

protein



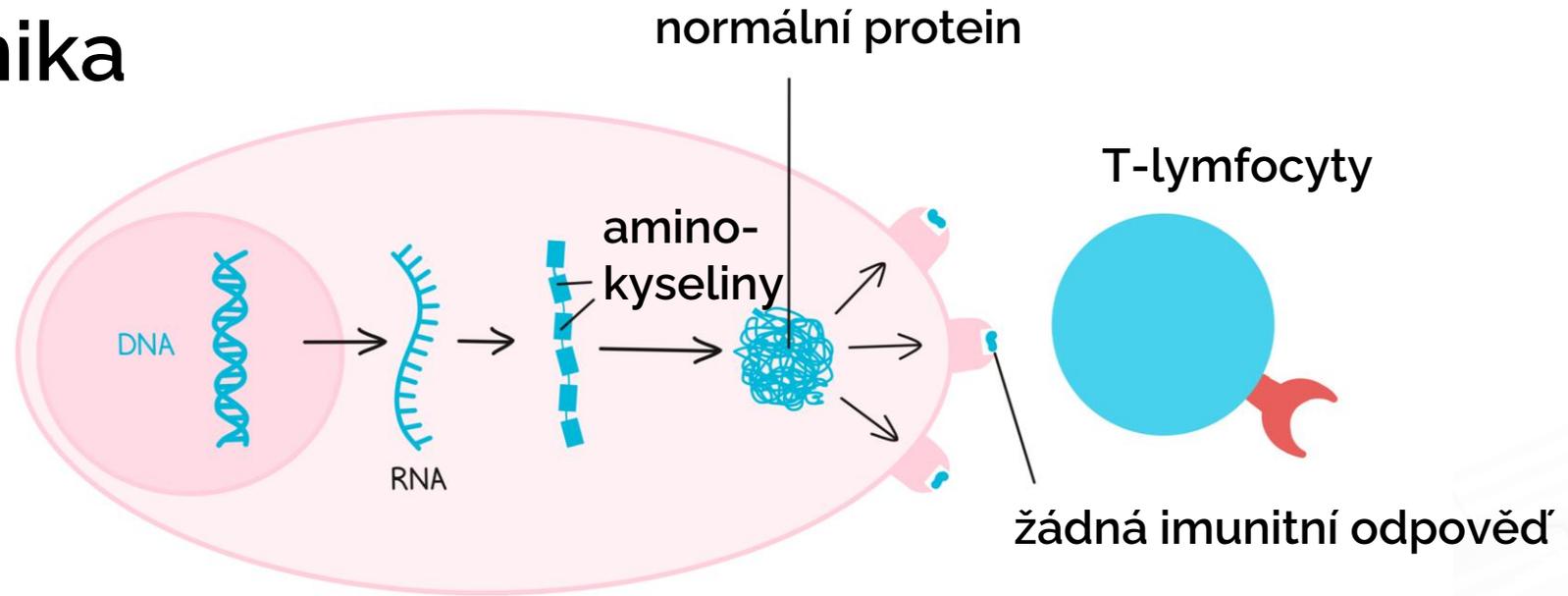


# Proteomika a hmotnostní spektrometrie

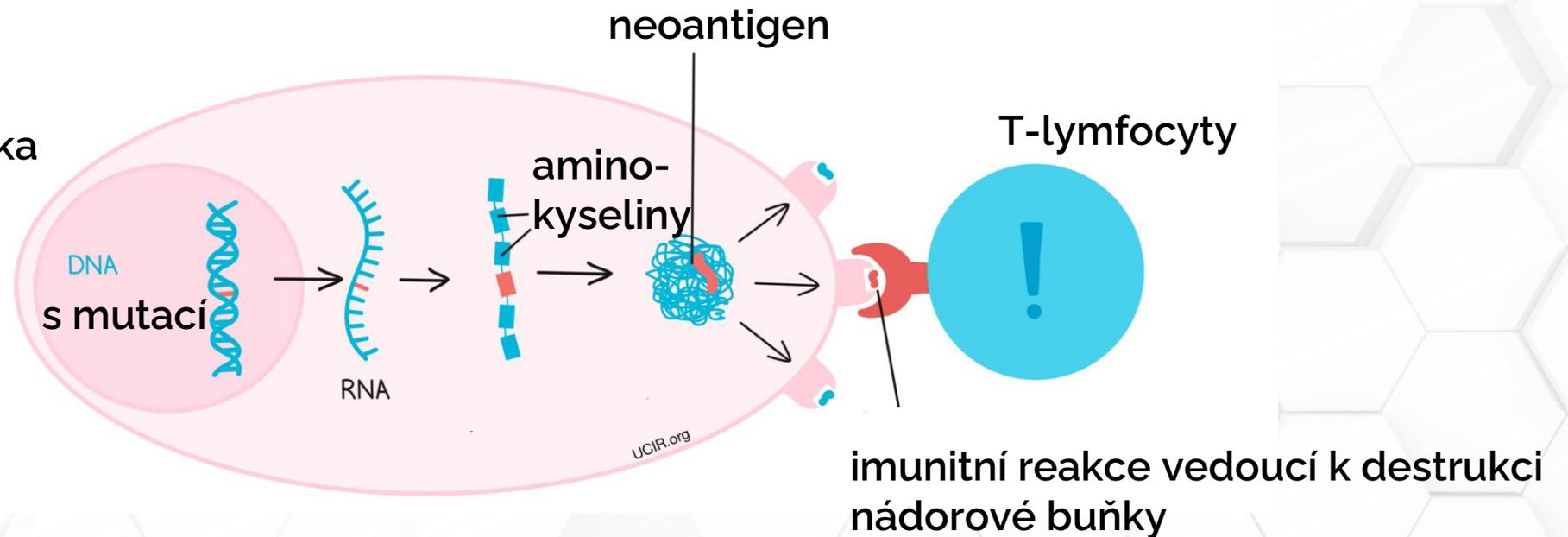


# Imunopeptidomika

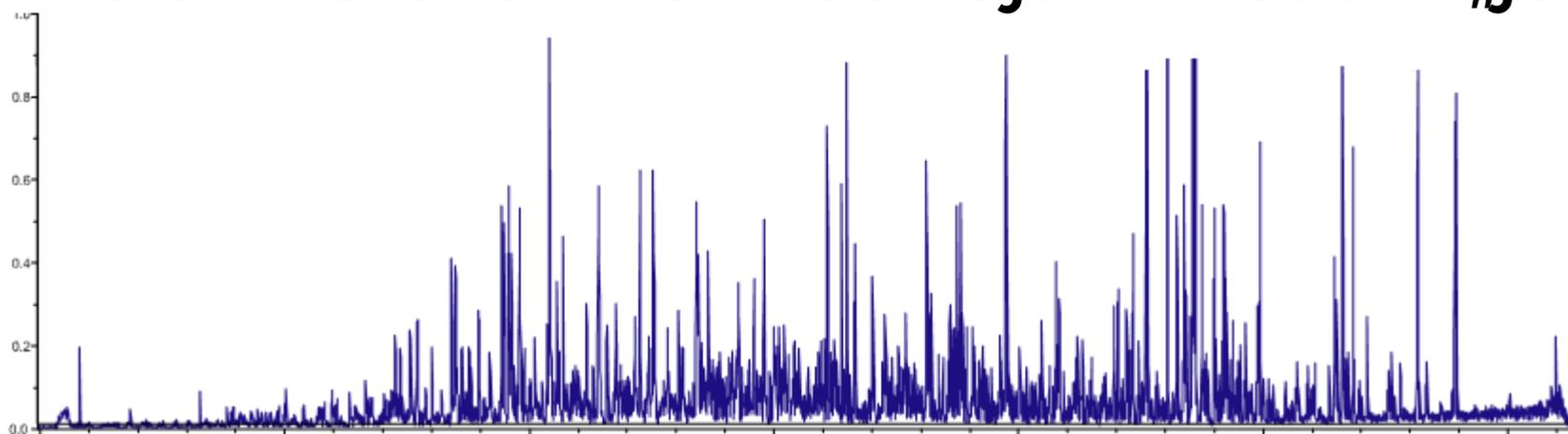
zdravá buňka



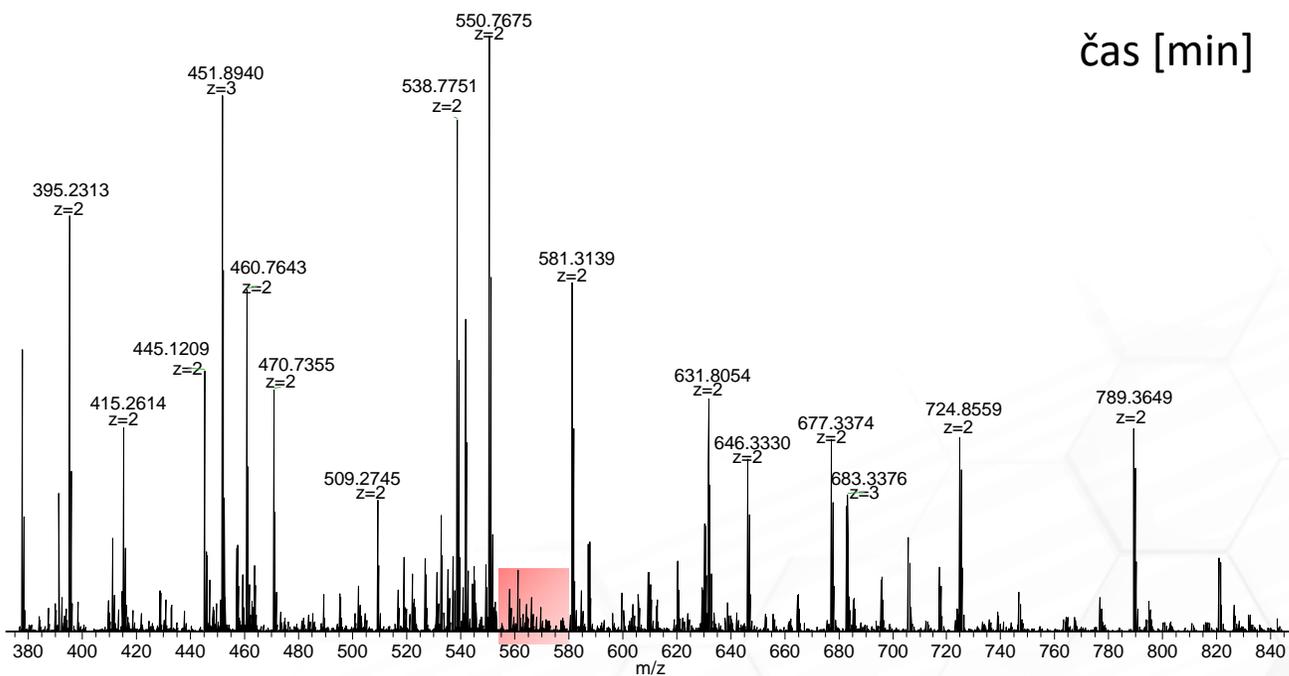
nádorová buňka



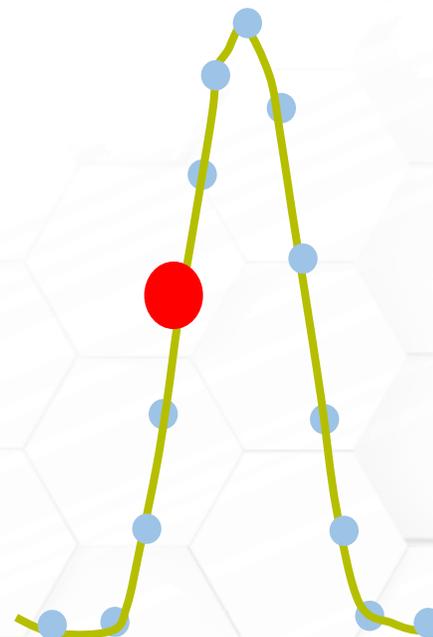
# Potřeba efektivních nástrojů k hledání „jehly“



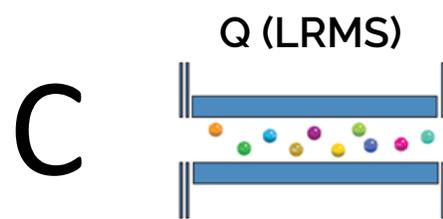
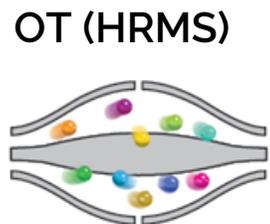
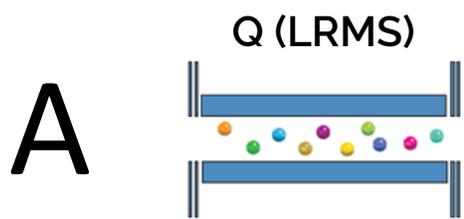
čas [min]



m/z



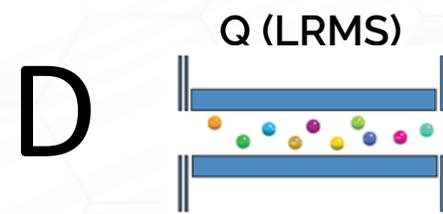
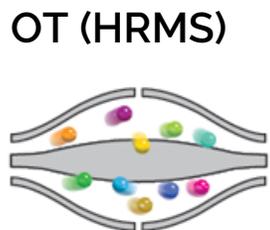
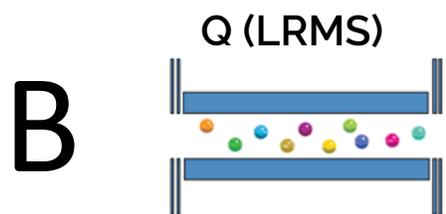
# Rozvoj instrumentace hmotnostní spektrometrie



OT (HRMS)



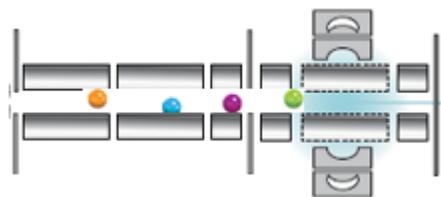
OT (HRMS)



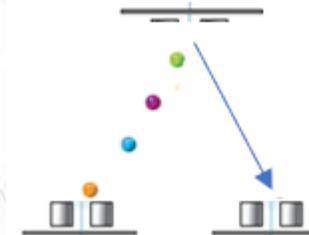
OT (HRMS)



LIT (LRMS)



TOF (HRMS)



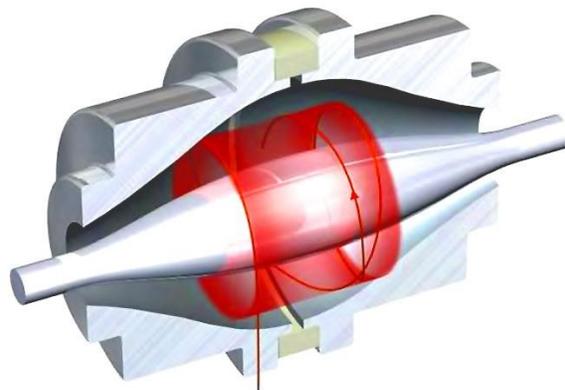


pragolab

pragolab

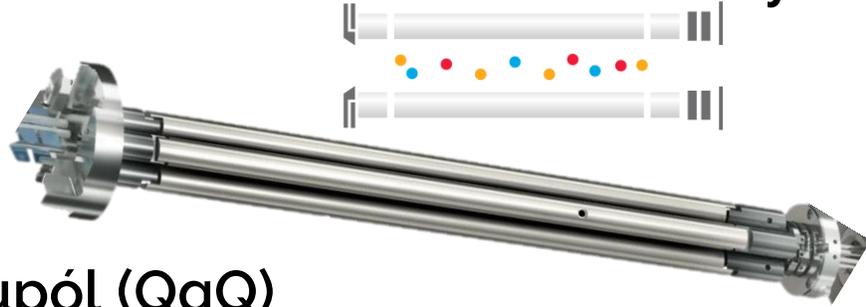
„Hvězdné“ hybridní MS

Roman Hájek



# Hmotnostní spektrometry s nízkým rozlišením

Jednoduchý kvadrupól (Q)



ISQ EM



ISQ EC

Trojítý kvadrupól (QqQ)



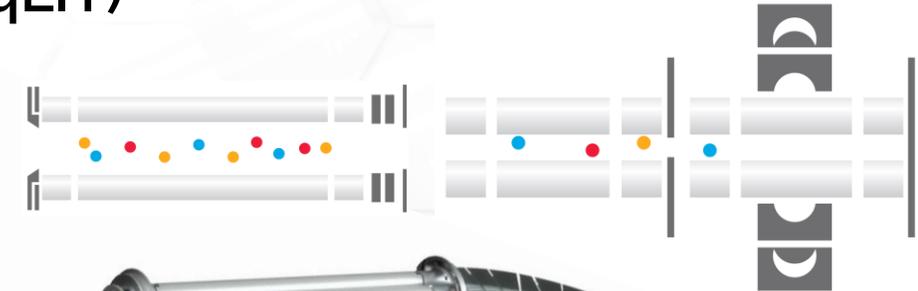
TSQ Altis Plus

TSQ Fortis Plus

TSQ Quantis Plus



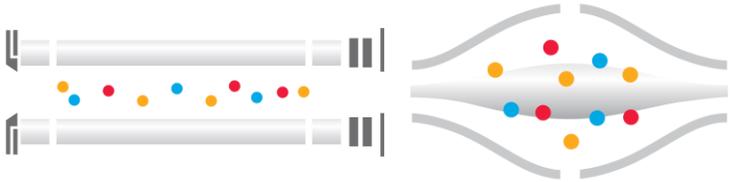
Kvadrupól s lineární iontovou pastí (QqLIT)



Stellar

# Hmotnostní spektrometry s vysokým rozlišením

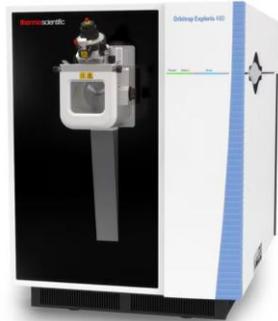
## Řada Orbitrap Exploris (QqOT)



Exploris 120

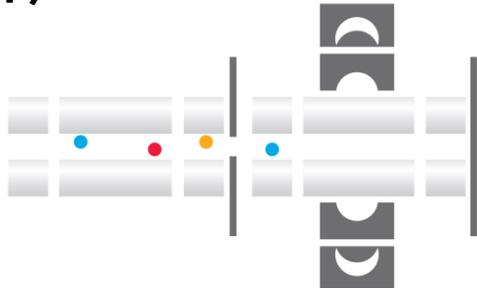


Exploris 240



Exploris 480

## Tribridy (QOTqLIT)



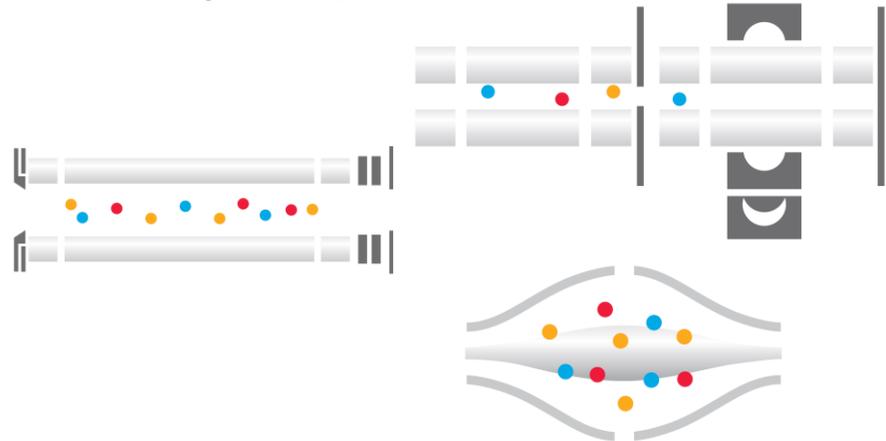
Orbitrap Eclipse



Orbitrap IQ-X

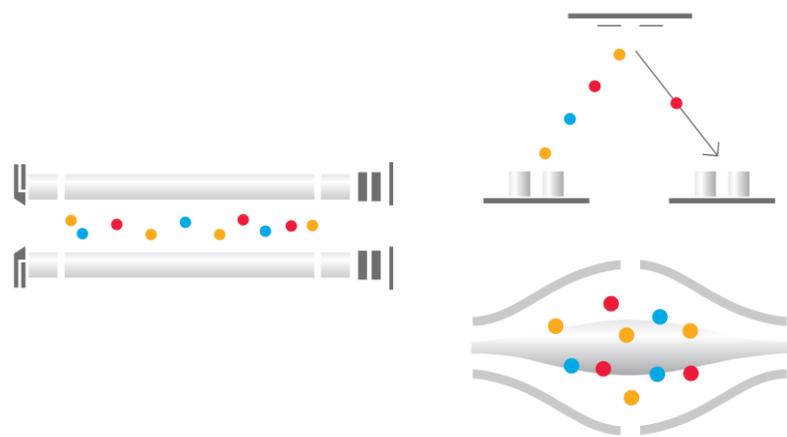
# Hmotnostní spektrometry s vysokým rozlišením rozlišením

## Tribridy (QqOTqLIT)



Orbitrap Ascend

## Tribridy (QOTqToF)



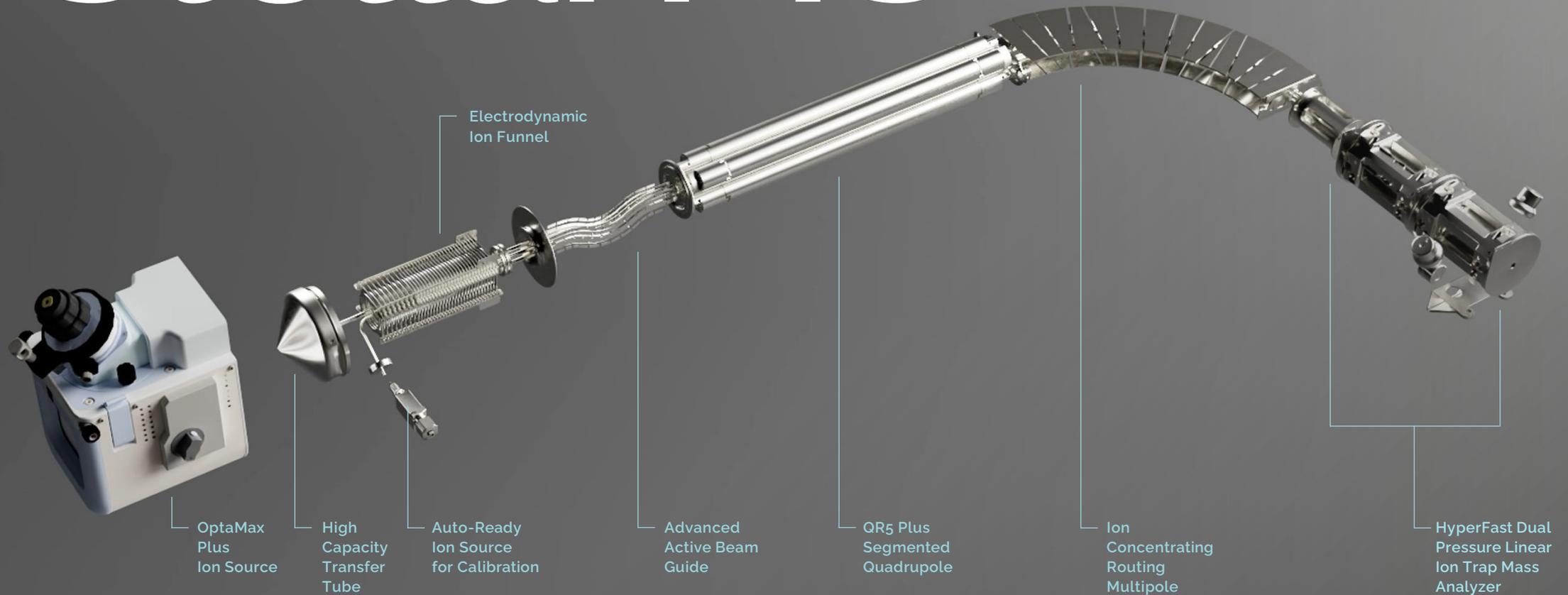
Orbitrap Astral



Uvedení

# Thermo Scientific™ Stellar™ hmotnostní spektrometr

# Stellar MS

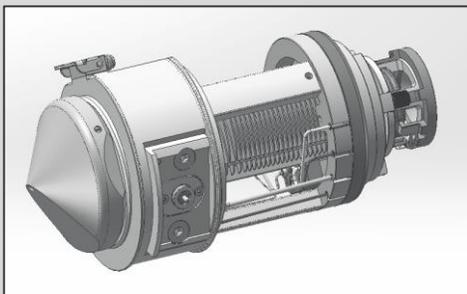


# Auto-Ready iontový zdroj pro kalibraci

Automatizované / vzdálené / předem naplánované kontroly a kalibrace systému

## Auto-Ready iontový zdroj

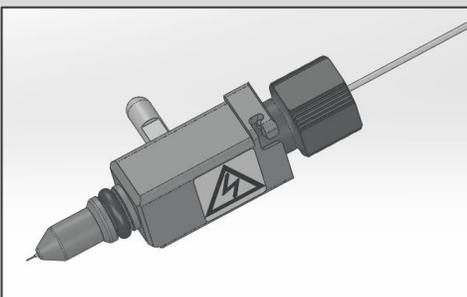
Samostatná trubice pro přenos iontů



Robustní systém



Dedikovaný emitér



**Status**

Self-check is scheduled to run every Wednesday at 12:00 AM in Check, Calibrate if Required mode.

**Polarity (+)    Polarity (+/-)**

Orbitrap Mass  
▶ Recommended Calibration: **5/2/2021**

System  
▶ Recommended Calibration: **5/9/2021**

Optional Calibrations

FlexMix Volume      Full (>= 70%)

**Calibration**

Mode: Check, Calibrate if required

Polarity: Positive and Negative

Type: Orbitrap Mass & System

**Optional Calibrations**

Easy-IC

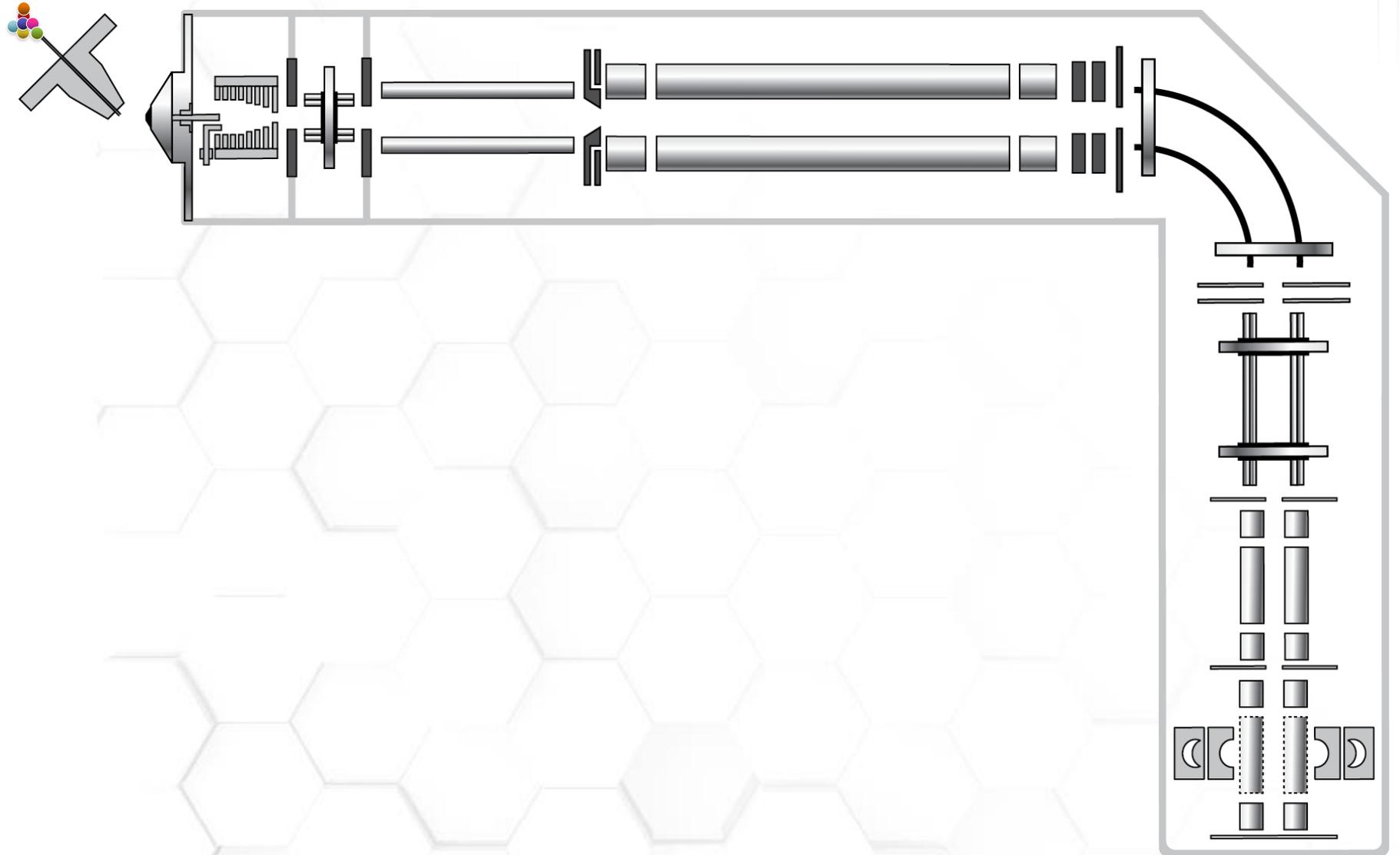
System self-check completed successfully at 01:59 PM on Feb 19

Passed

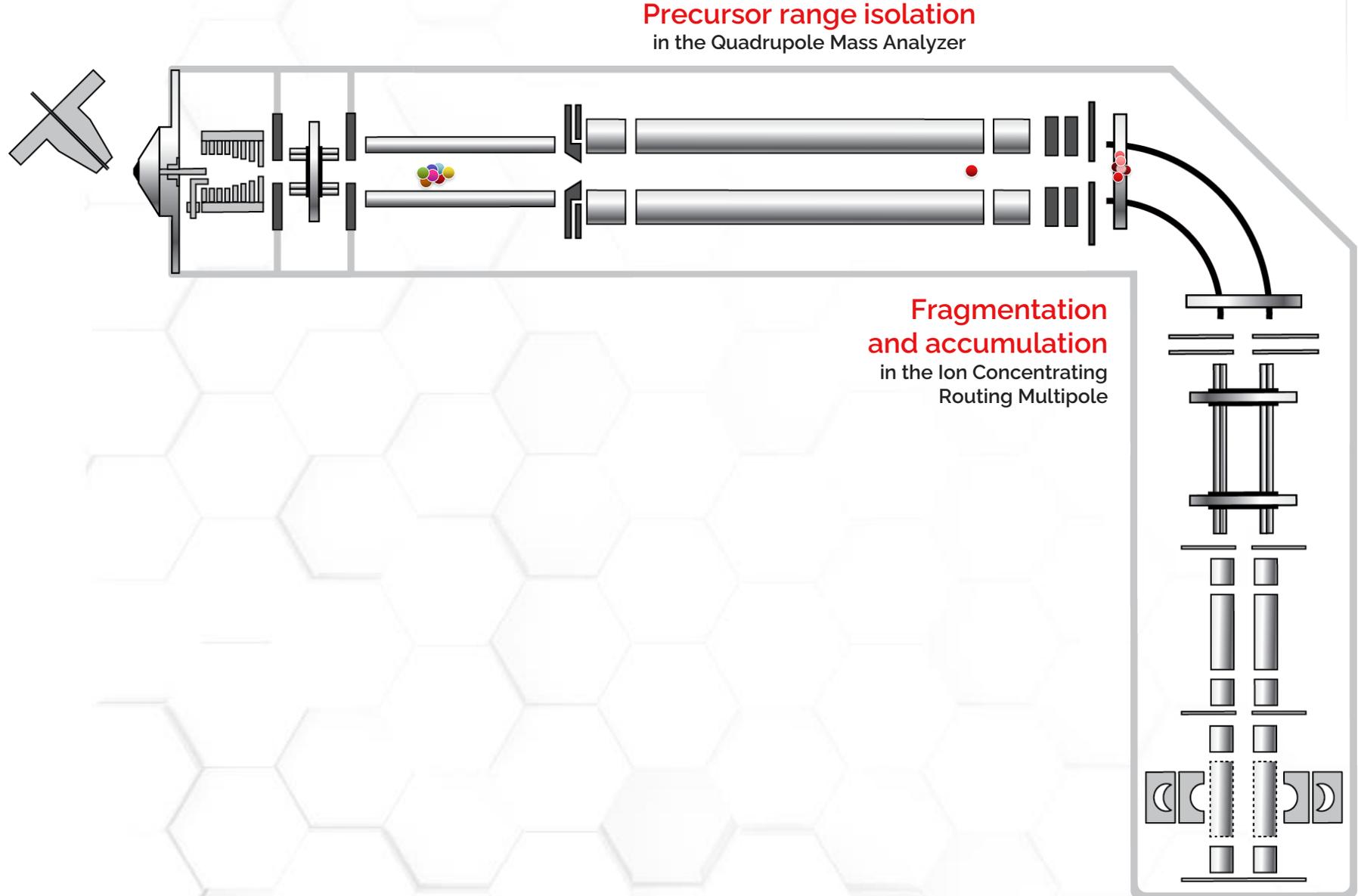


# Stellar hmotnostní spektrometr PRM akvizice pro MS<sup>2</sup> spektra

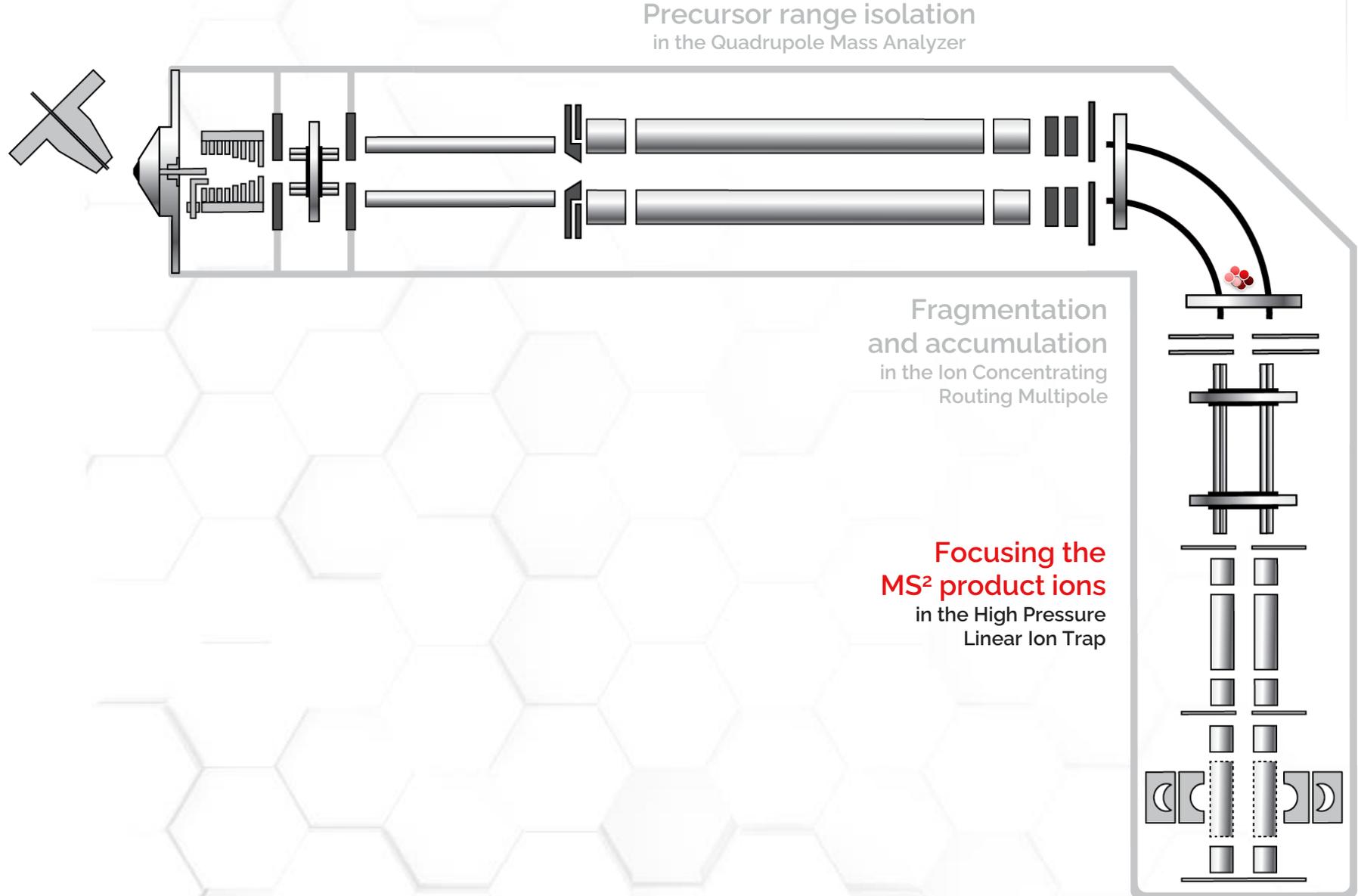
Coordinated control of ions  
in a step-wise manner  
In the Stellar mass spectrometer



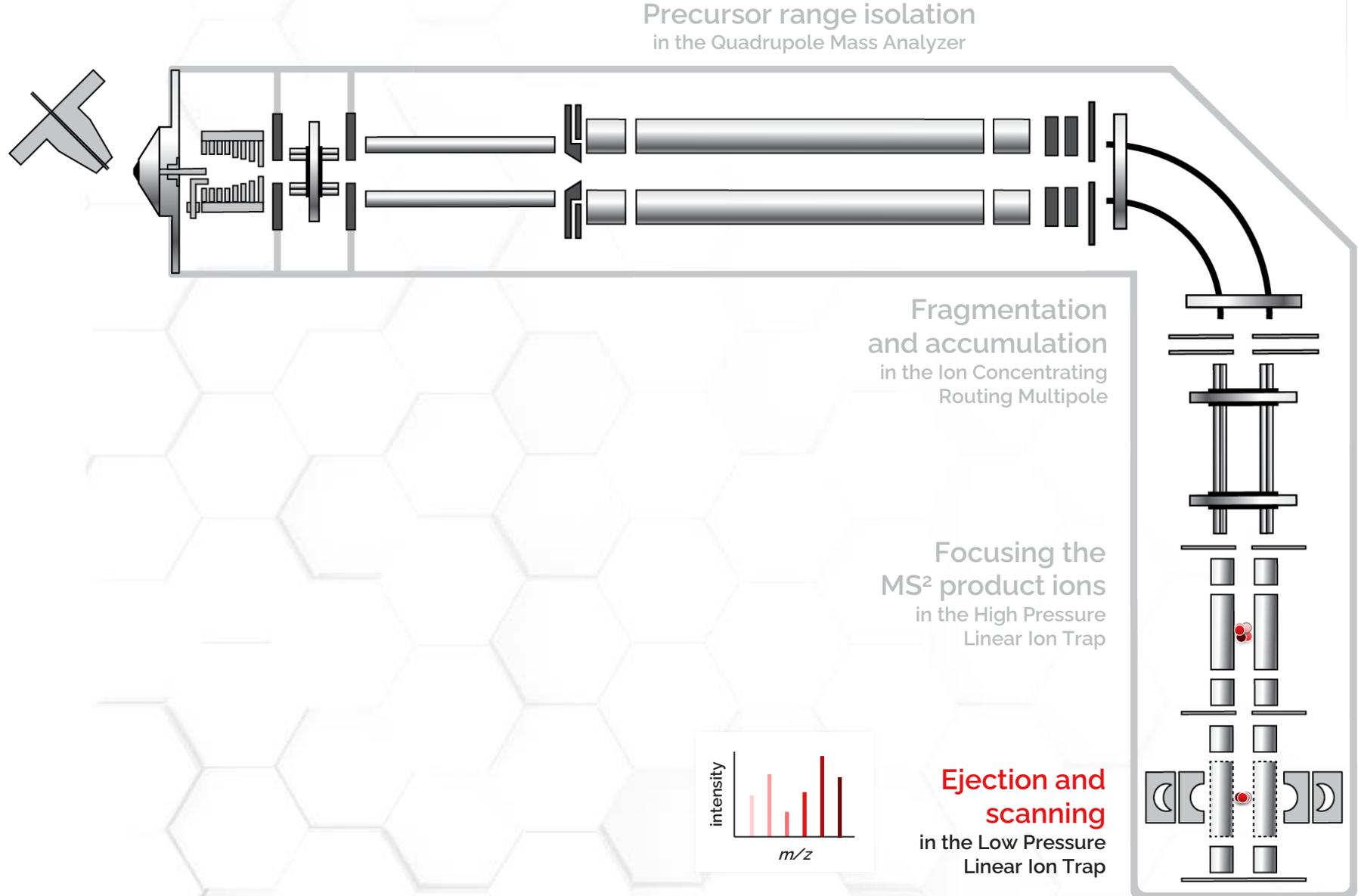
# Stellar hmotnostní spektrometr PRM akvizice pro MS<sup>2</sup> spektra



# Stellar hmotnostní spektrometr PRM akvizice pro MS<sup>2</sup> spektra

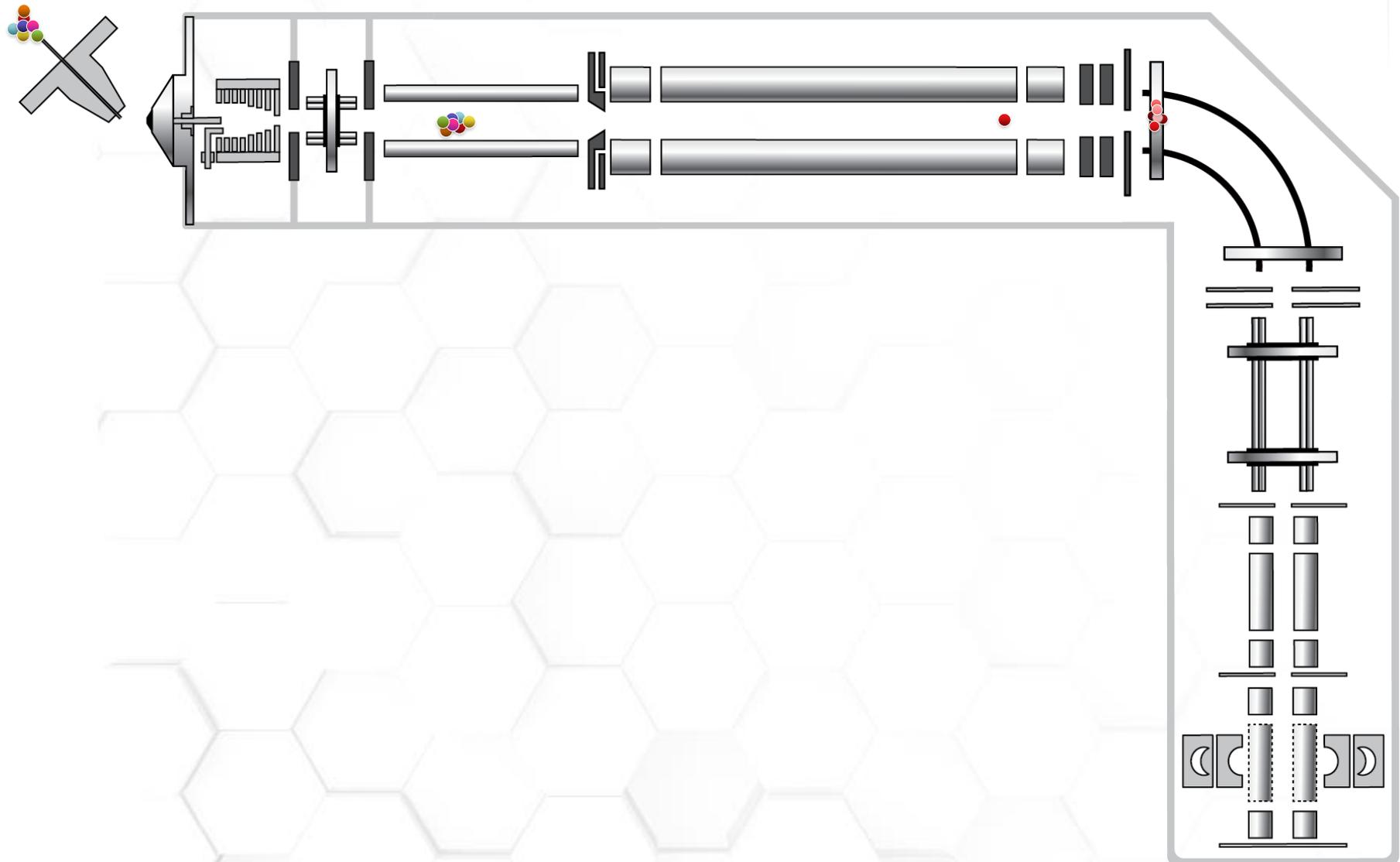


# Stellar hmotnostní spektrometr PRM akvizice pro MS<sup>2</sup> spektra



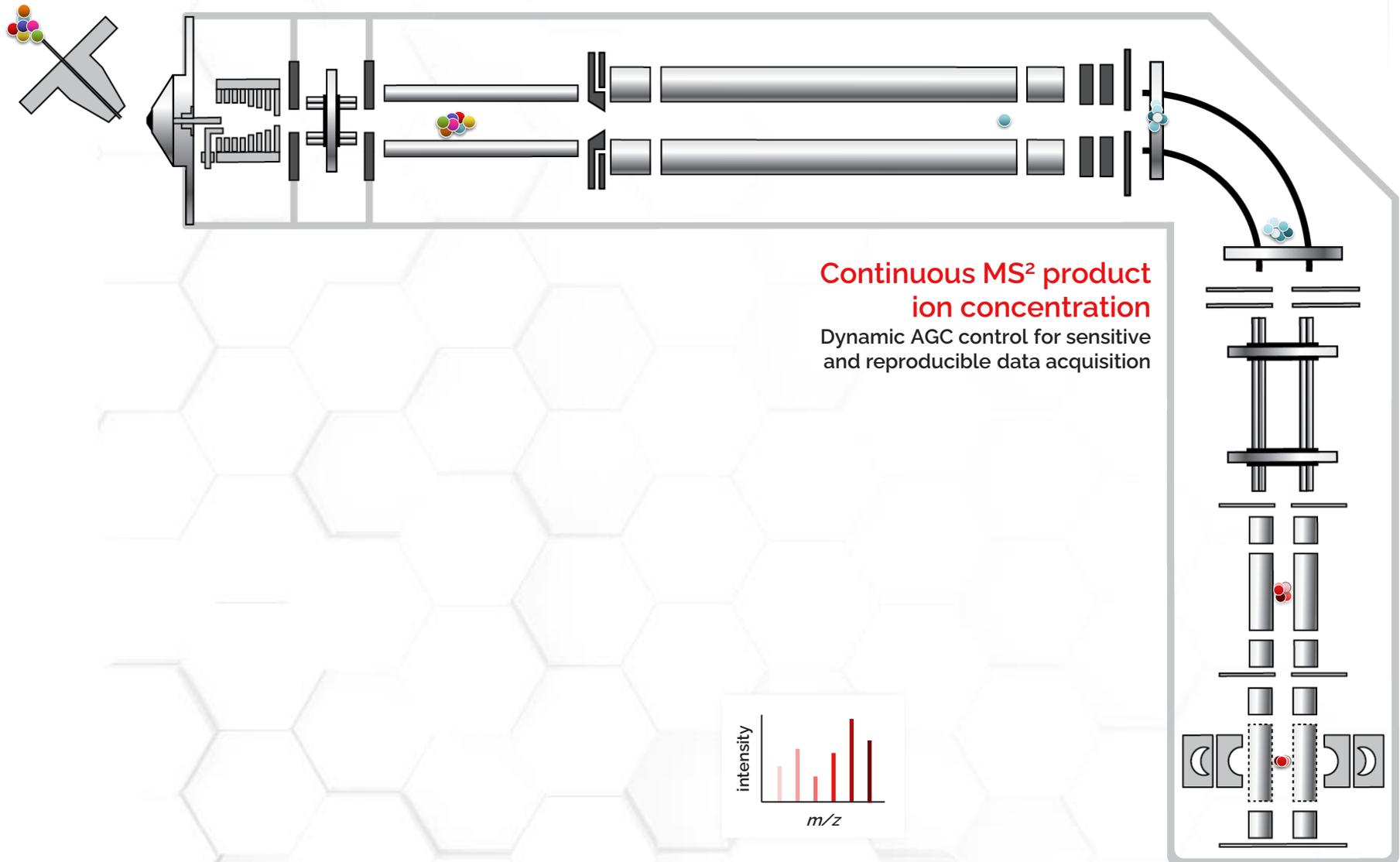
# Stellar hmotnostní spektrometr PRM akvizice pro MS<sup>2</sup> spektra

Increased ion utilization  
for faster MS<sup>2</sup> acquisition  
Synchronized dual ion packet  
processing with dynamic ion modulation

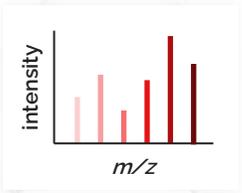


# Stellar hmotnostní spektrometr PRM akvizice pro MS<sup>2</sup> spektra

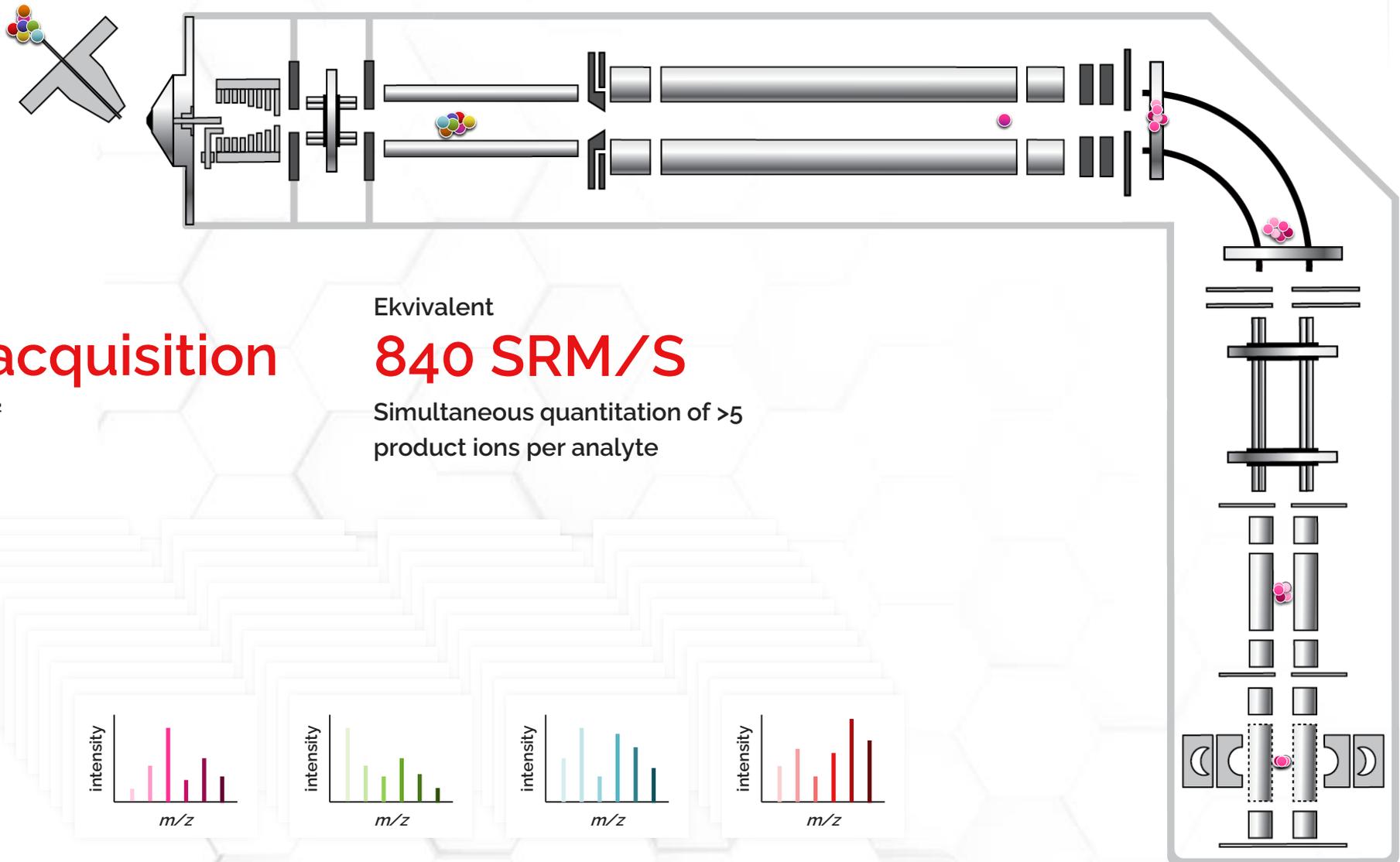
**Increased ion utilization  
for faster MS<sup>2</sup> acquisition**  
Synchronized dual ion packet  
processing with dynamic ion modulation



**Continuous MS<sup>2</sup> product  
ion concentration**  
Dynamic AGC control for sensitive  
and reproducible data acquisition



# Stellar hmotnostní spektrometr PRM akvizice pro MS<sup>2</sup> spektra



**140 Hz**

Scan rate

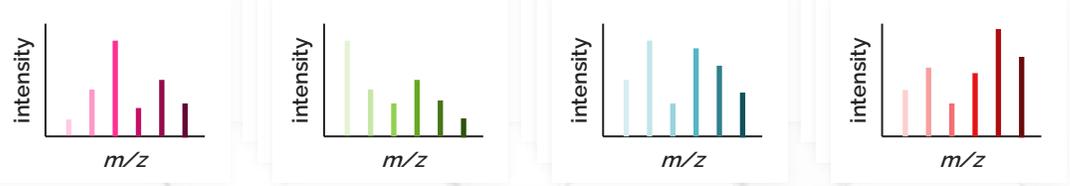
**PRM acquisition**

Full scan MS<sup>2</sup>

Ekvivalent

**840 SRM/S**

Simultaneous quantitation of >5 product ions per analyte



# Jak pracuje PRM akvizice pro MS<sup>3</sup> spektra

Stellar MS

PRM akvizice pro **MS<sup>3</sup>** spektra



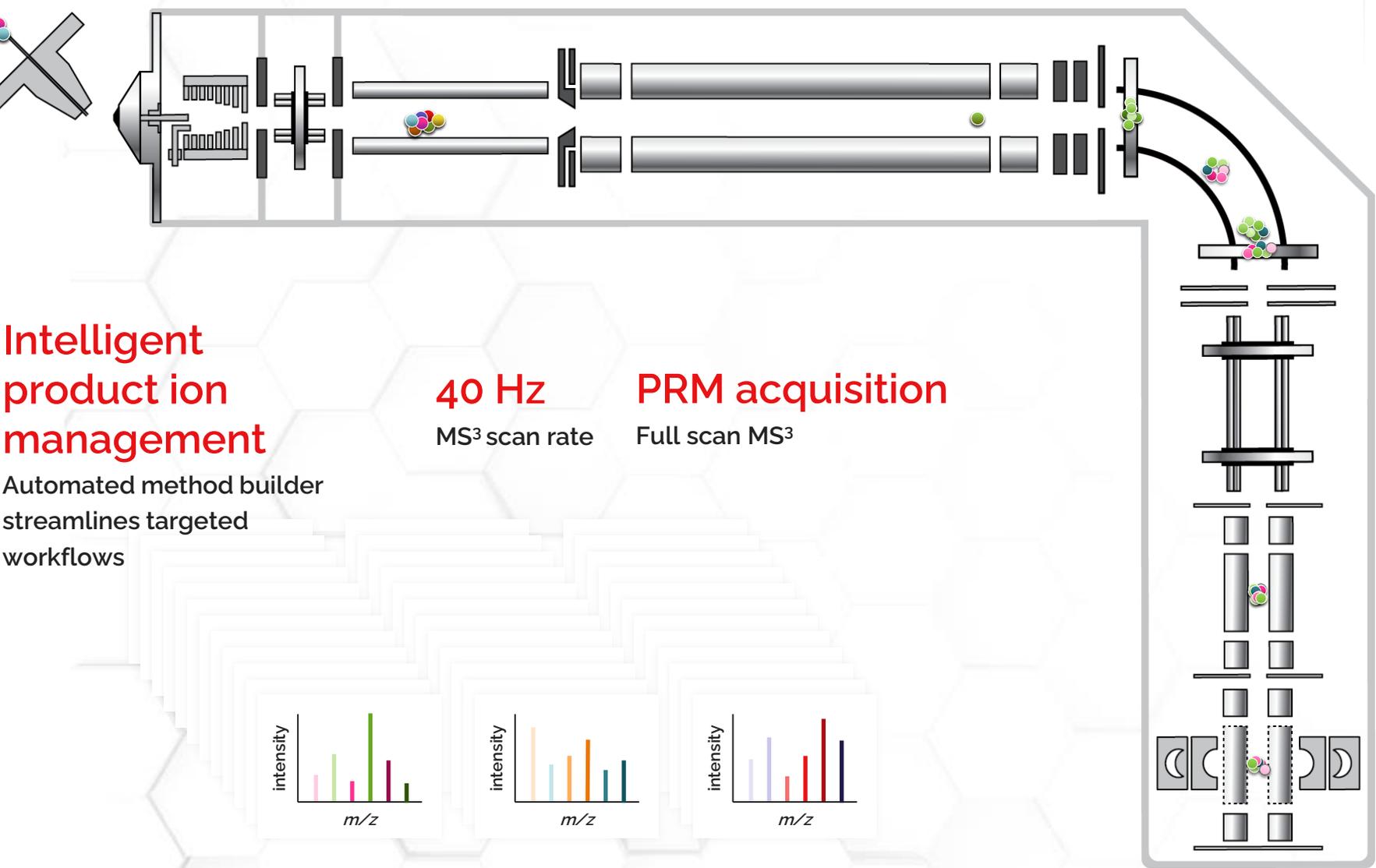
# Jak pracuje PRM akvizice pro MS<sup>3</sup> spektra

## Maintain high ion utilization for fast MS<sup>3</sup> acquisition

Synchronized dual ion packet processing with dynamic ion modulation

## Synchronous precursor selection

Increase specificity, selectivity, and sensitivity

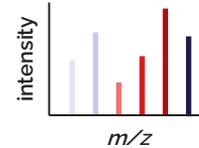
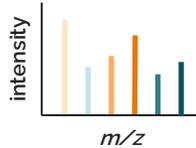
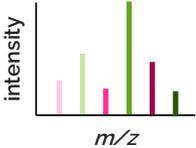


## Intelligent product ion management

Automated method builder streamlines targeted workflows

40 Hz MS<sup>3</sup> scan rate

PRM acquisition Full scan MS<sup>3</sup>

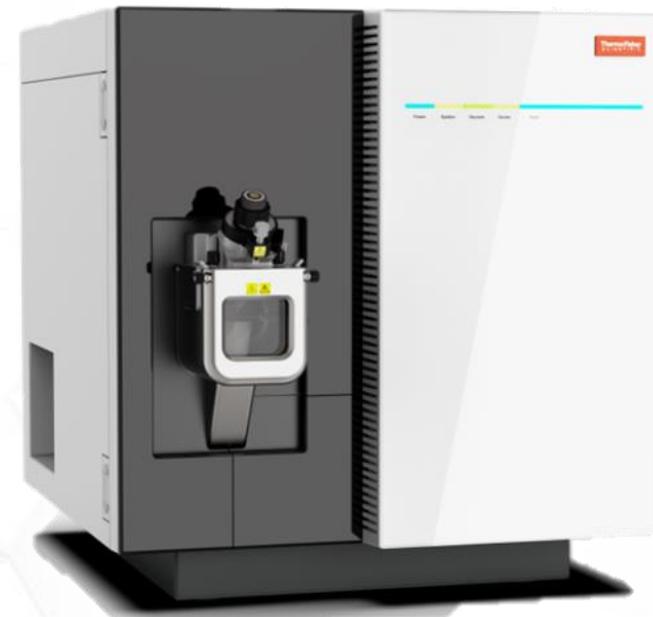


# Stellar

Nový hybridní hmotnostní spektrometr poskytující cílené experimenty nové generace

## Stellar – patří do skupiny nízko rozlišujících hmotnostních spektrometrů

- Hybridní hmotnostní spektrometr s konstrukčními prvky kvadrupólového hmotnostního analyzátoru a technologií lineární iontové pasti
- Poskytuje vysokou citlivost při extrémní rychlosti měření
- Možnost měření:
  - full scan produktových iontů pro každý prekurzor (PRM)
  - MS<sup>n</sup>
- HCD nebo CID fragmentace
- Inteligentního sběru dat (Adaptive RT)



Introducing the

# Thermo Scientific<sup>TM</sup> Orbitrap<sup>TM</sup> Astral<sup>TM</sup>

MASS SPECTROMETER

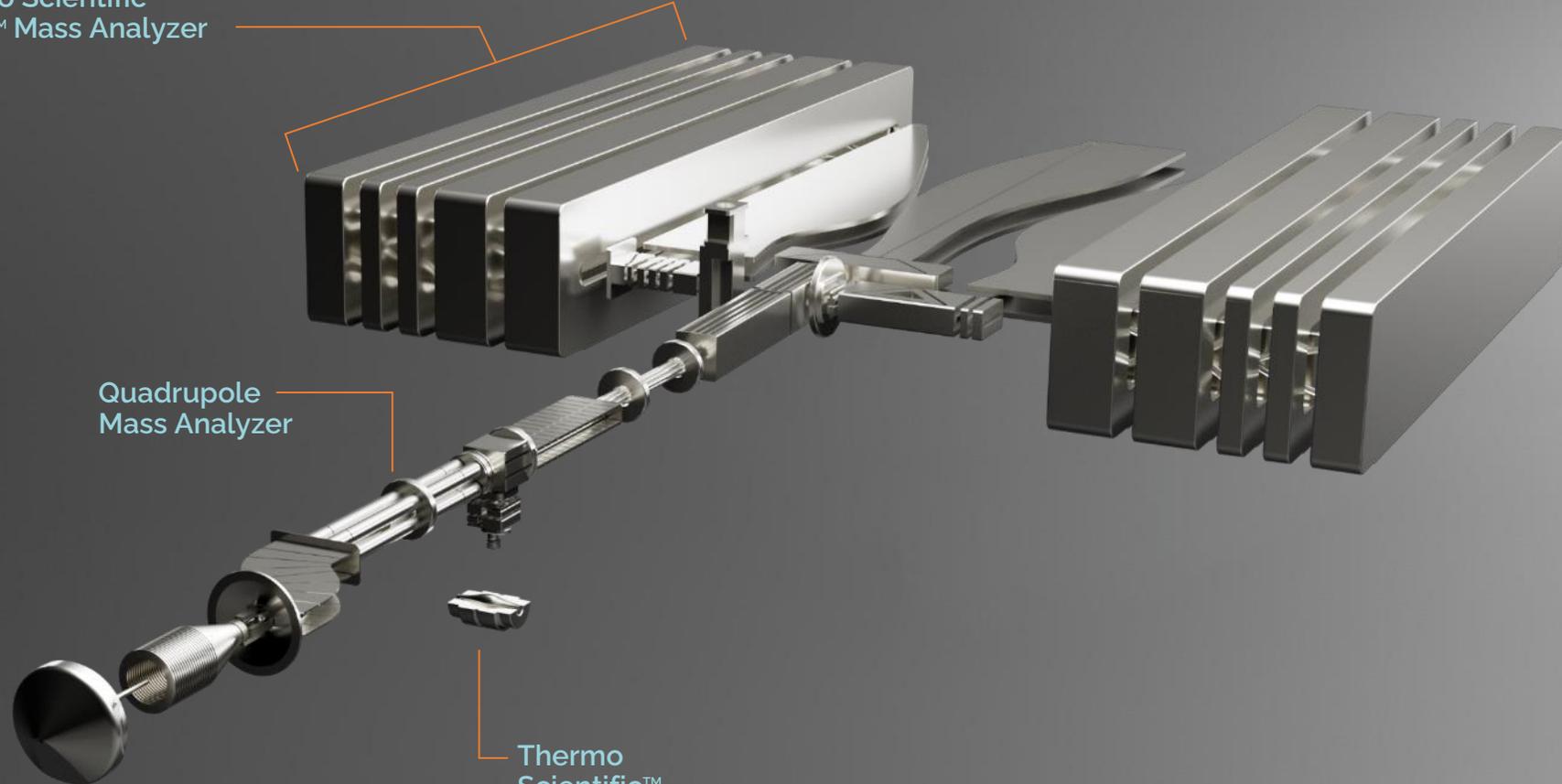


# The Orbitrap Astral MS

Thermo Scientific™  
Astral™ Mass Analyzer

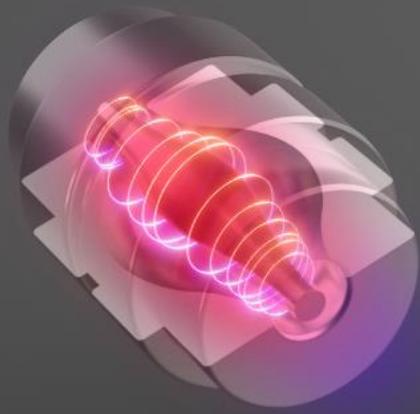
Quadrupole  
Mass Analyzer

Thermo  
Scientific™  
Orbitrap™ Mass  
Analyzer



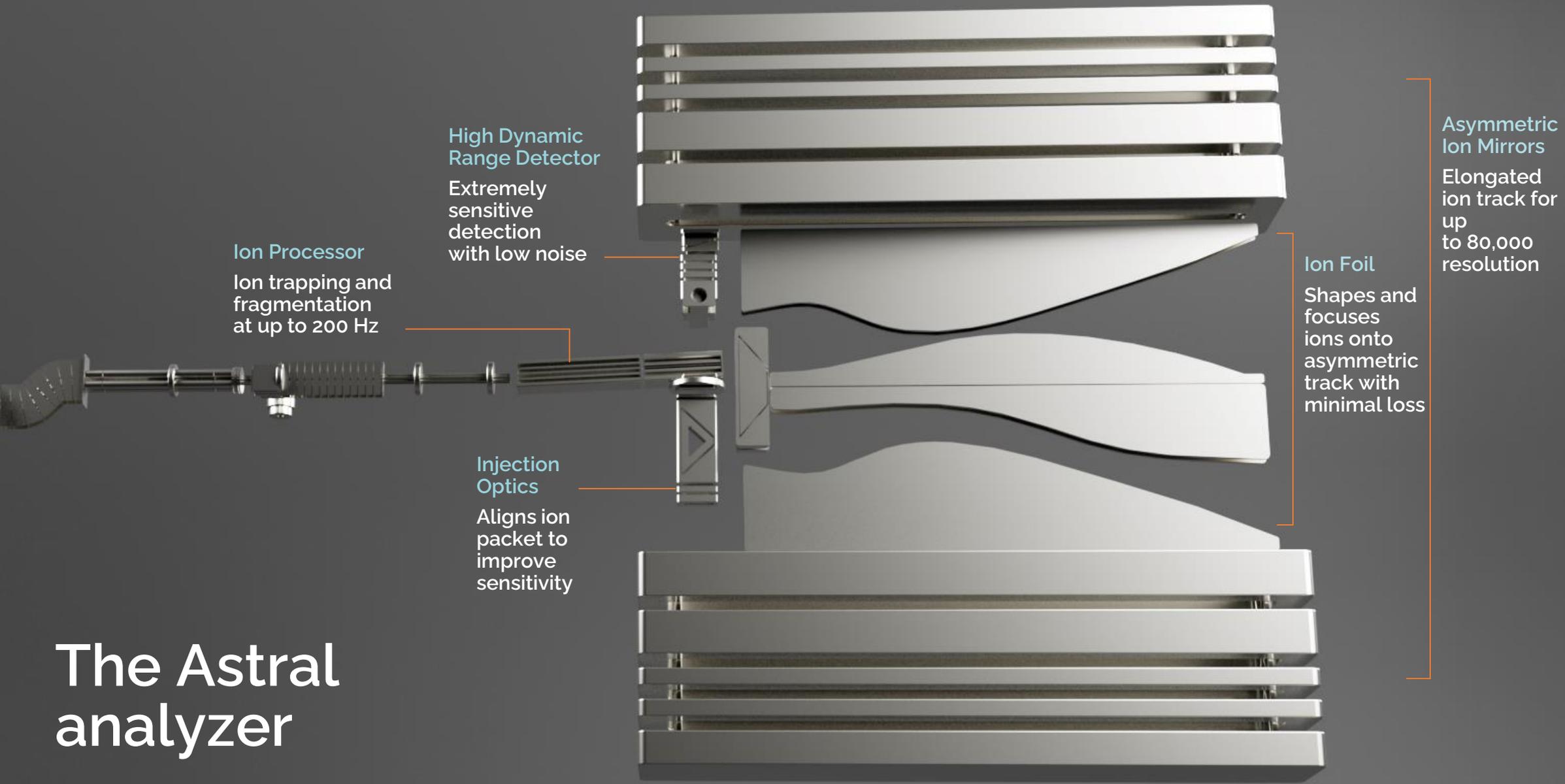


**Ion Routing Multipole**  
Efficient ion trapping and HCD fragmentation  
Facilitates parallelization



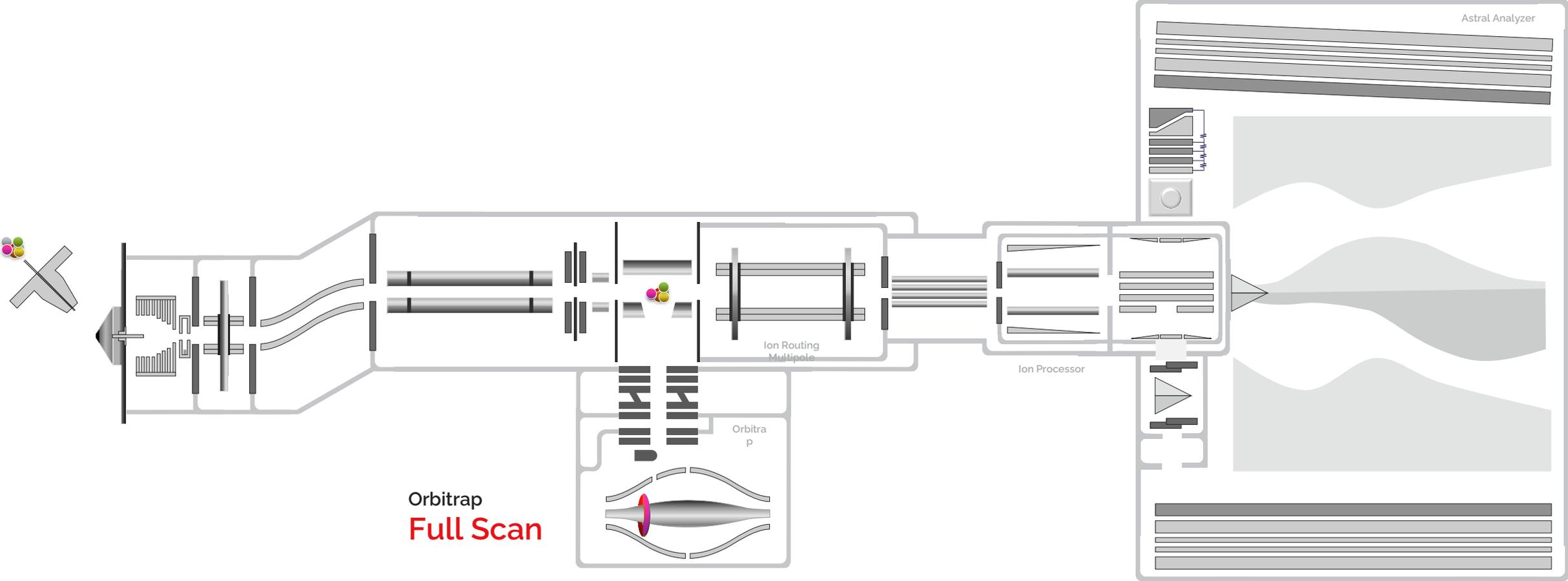
**Ultra-High-Field Orbitrap**  
High resolution up to 480,000  
Scan speeds up to 40 Hz  
High dynamic range  
High mass accuracy

# The Orbitrap analyzer

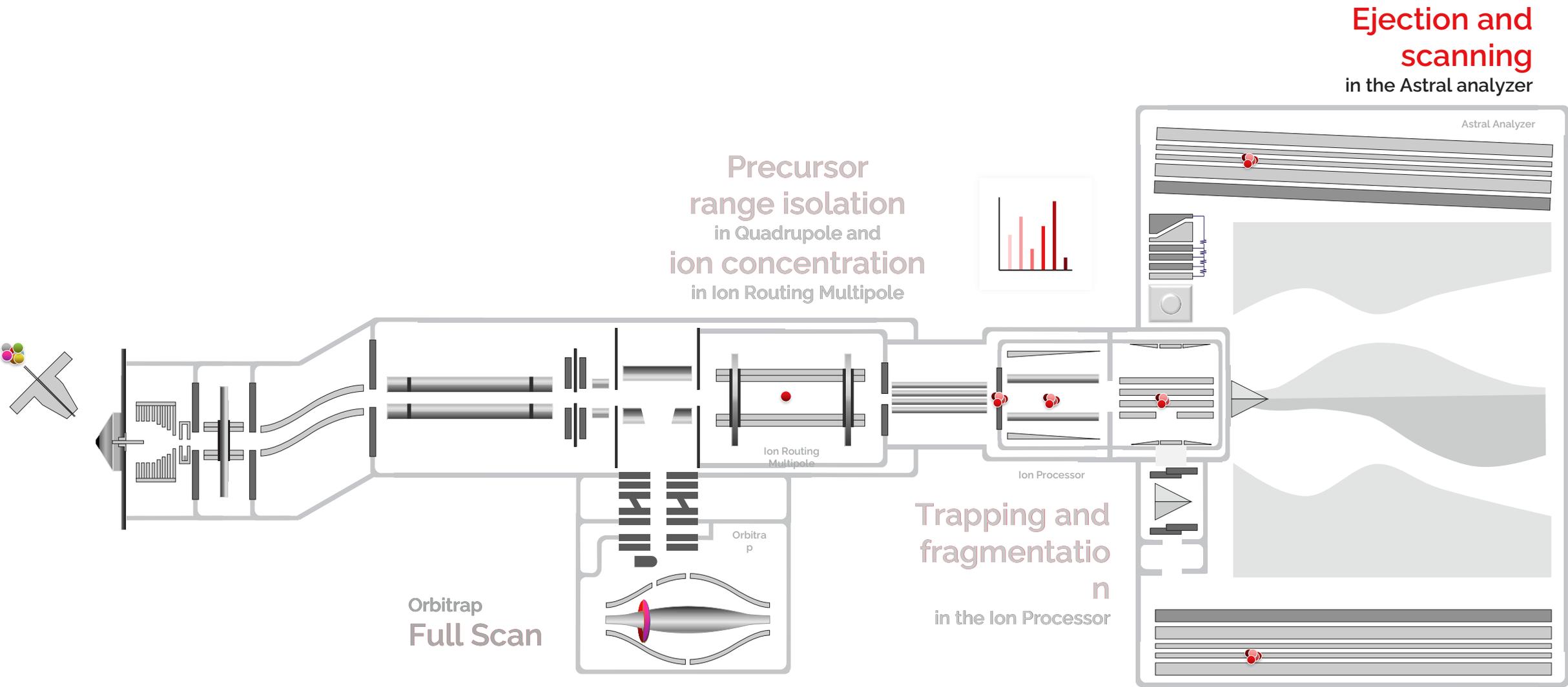


# The Astral analyzer

# Orbitrap Astral mass spectrometer HR-DIA scan



# Orbitrap Astral mass spectrometer HR-DIA scan



Ejection and scanning  
in the Astral analyzer

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

Trapping and fragmentation  
in the Ion Processor

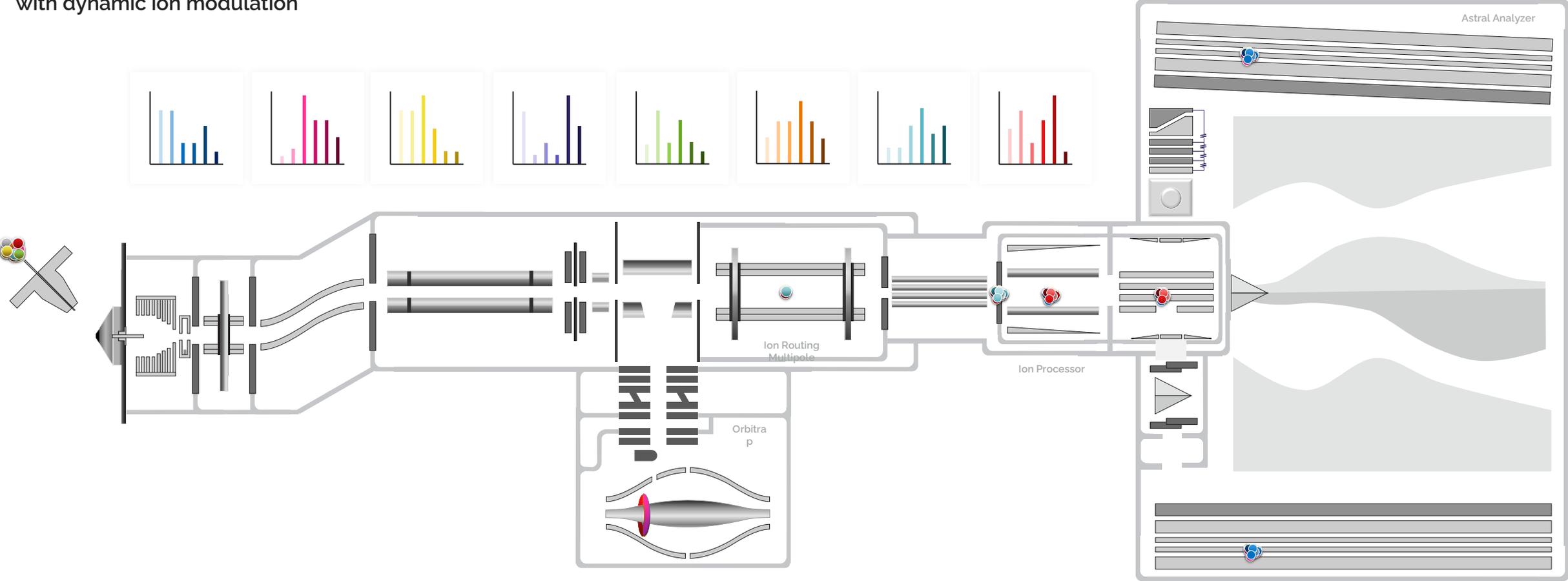
Orbitrap Full Scan

Astral Analyzer

# Orbitrap Astral mass spectrometer HR-DIA scan

## 5 ion packets

simultaneously processed in parallel  
with dynamic ion modulation



# Orbitrap Astral mass spectrometer HR-DIA scan

**200 Hz**

scan rate

**240K**

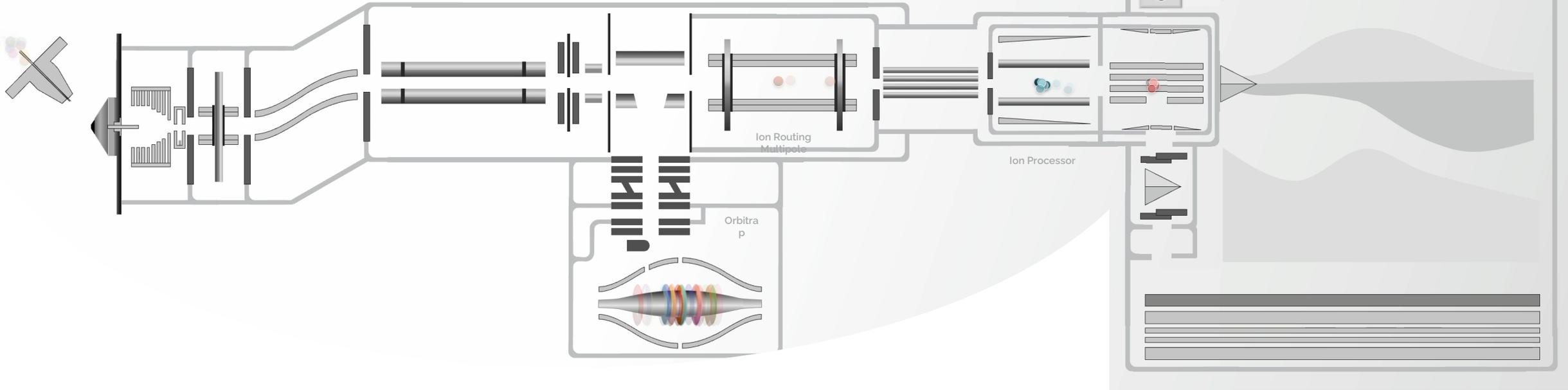
resolution full scan  
in 0.5 second

**100 MS<sup>2</sup>**

scans in the Astral analyzer  
in 0.5 second

**56x faster**

in real-time than shown



Děkuji za pozornost

