A (Ultra-)High Resolving Time-of-Flight Mass Spectrometer with MS^N Capability

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Introduction

Common compact mass spectrometers are typically limited to low or medium mass resolving power. To overcome this limitation, a mobile multiple-reflection time-of-flight mass spectrometer (MR-TOF-MS) has been developed [1,2].

It allows for sub-ppm accuracy with (ultra-)high mass resolving power in a compact size and is capable of resolving isobars.

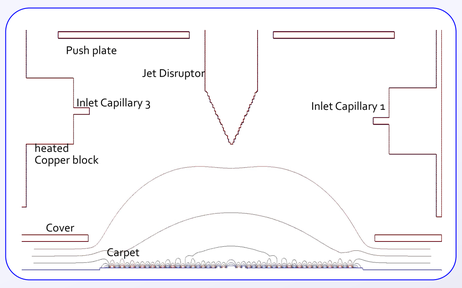
The device offers multiple-stage tandem mass spectrometry with very high mass resolving power in every stage using the novel technique of mass-selective ion-trapping [3,4].

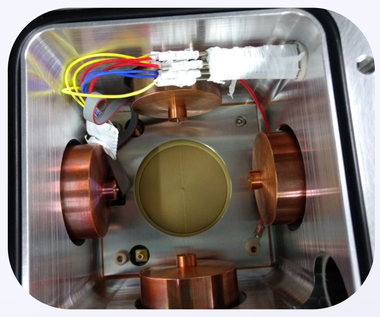
Atmospherical Pressure Inlet

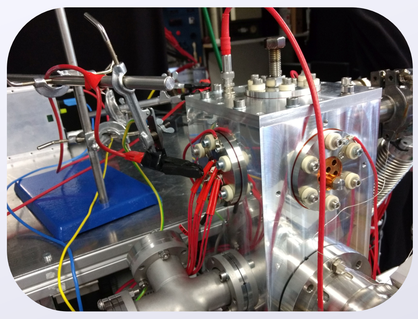
A new atmospherical pressure inlet (API) was designed, build and put into operation.

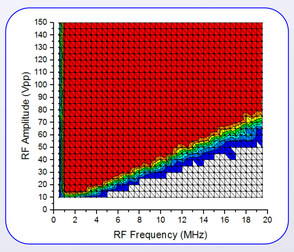
Features

- up to 4 parallel inlet capillaries
- individually heated inlet capillaries
- high transmission
- mass selective carpet
- online adjustable jet disruptor
- online exchangeable commercial capillaries
- compatible with commercial ion sources

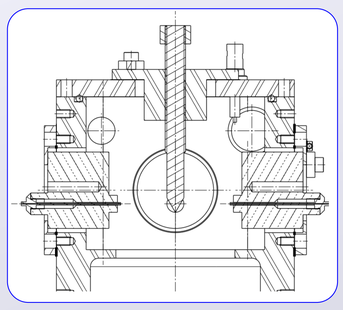








Simulations
top: ion flight path
bot: carpet transmission of 195 u

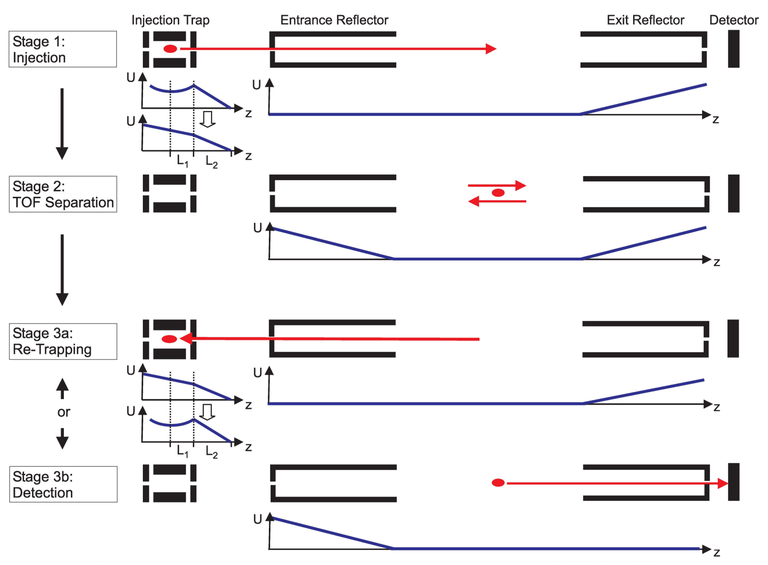


Design and Setup
of the new API
top: inside of upper chamber
mid: outside with n-ESI
bot: Design concept

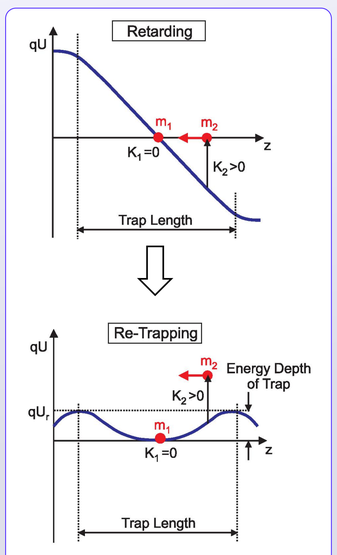
Re-Trapping

Work flow

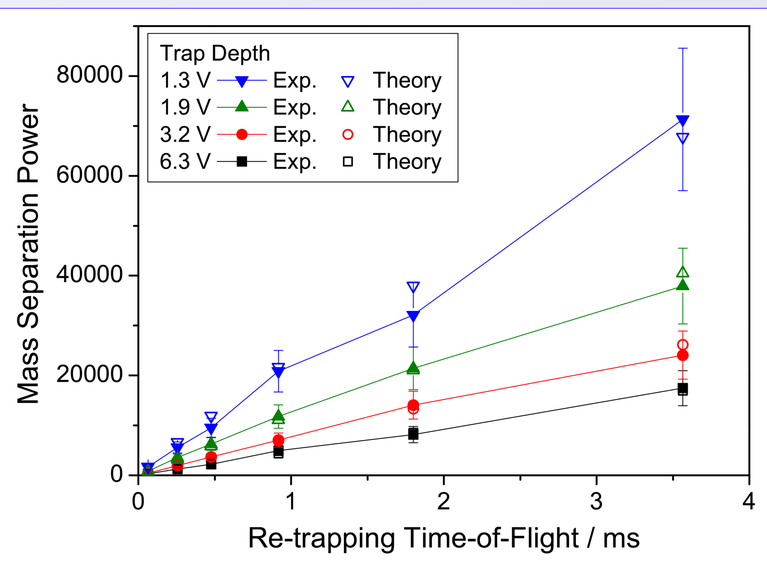
1. Ions are cooled and injected into the analyzer
2. Mirrors reflect ions to increase flight path
   ⇒ Long flight paths disperse ions in time
3a. Ions are re-trapped in the RFQ-Trap
   ⇒ CID breaks up molecules by exciting ion's macro motion
3b. Ions are injected into the analyzer again



Stages of mass selective re-trapping of ions at an MR-TOF-MS [4]



Trap potentials for retrapping [4]



Separation power in dependence of retrapping time [3,4]

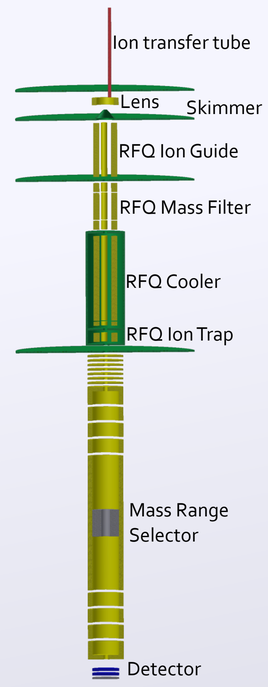
Features

- Precursor selection in the same analyzer as themeasurement
- Re-trapping (precursor selection) resolving power up to 70 000

Setup



The mobile MR-TOF-MS outside the II. Physical Institute's building.



Atmospheric Pressure Interface (API)
1 bar ... 10^{-2} mbar

Beam Preparation System
10^{-2} mbar ... 10^{-4} mbar

Analyzer
10^{-7} mbar

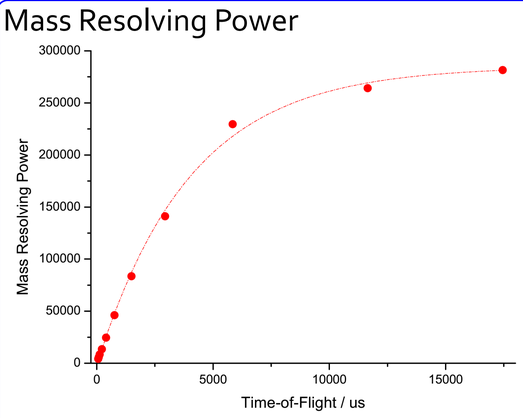
Schematic layout of the MR-TOF-MS [3]

Performance

Repitition rate: 1 kHz
Atmospheric Ion Source
Mobile setup: 0.8 m³

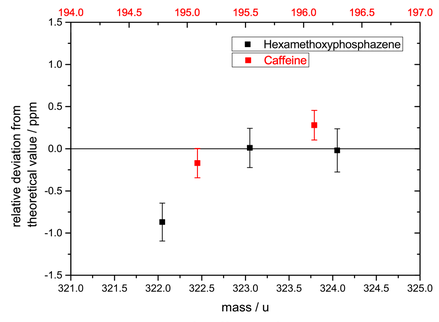
Setup Characterization

Mass Resolving Power



Mass Resolving Power of up to 300 000 has been reached [3]

Mass Measurement Accuracy:



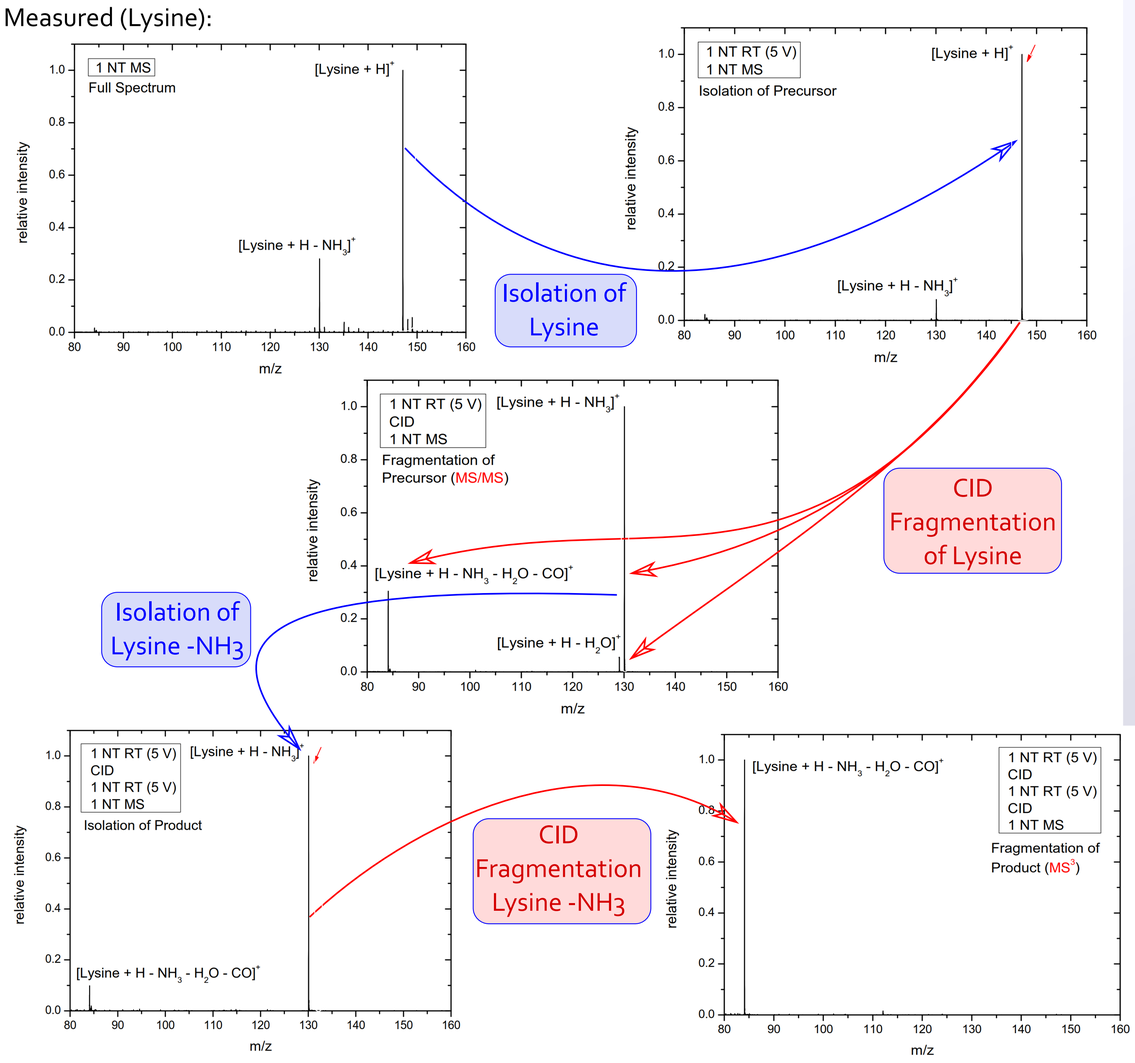
Relative Mass Accuracy of Caffeine of < 1 ppm [3]

Features

- Relative Mass Accuracy < 0.5 ppm (Caffeine)
- Mass Resolving Power up to 300 000
- Detection Limit of < 10^{-9} mol/l (Arginine)

MS^3 of Lysine

Lysine was measured, isolated and dissociated (CID).
Lysine - NH_3 ($C_6H_{12}N_1O_2$) at m = 130 u was again isolated and dissociated.



MS³ of Lysine [3]: 1) Full spectrum, 2) Isolation of precursor, 3) CID, 4) Isolation of product, 5) Fragmentation of product

Acknowledgements and Contact

[1] T. Dickel et al., Nucl. Instrum. Methods B 317 (2013) 779
[2] J. Lang, PhD thesis, 2016, JLU Gießen
[3] W. Lippert, PhD thesis, 2016, JLU Gießen
[4] T. Dickel et al., J. Am. Soc. Mass Spectrom. 28(2017) 1079
[5] T. Dickel et al., Int. J. Mass Spectrom. 412 (2017) 1-7

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