Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer

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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].

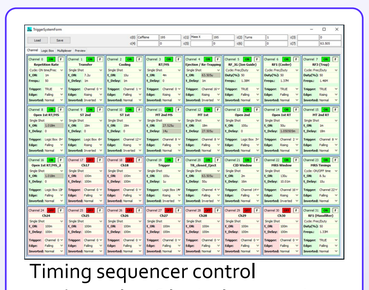
Hardware Control and Data Acquisition

A Software was designed and developed to improve data aquisition, analysis and hardware control.

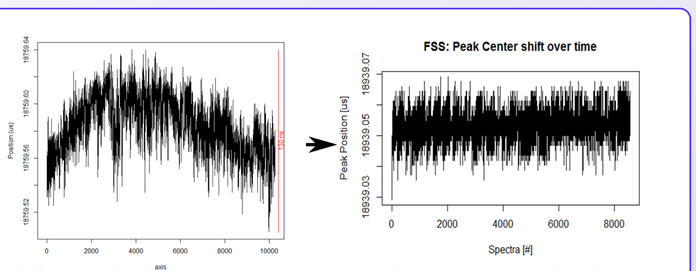
Hardware control
- Full control and preview of RFQ time sequencer via fpga board
- Optimizer can access applied voltages and time sequencer
- Feedback software stabilizer keep flight times stable

Data Acquisition
- Support of parallel ADCs/TDCs for increased dynamic range
- Enables long term measurement with auto-save feature

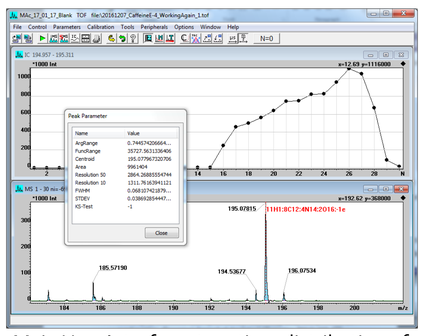
Analysis
- Online Analysis tools and filters
- Peak detection and multiple turn calibration
- intelligent Peak identification (NuBase13)
- TDC dead time correction tools
- RServe Connection to the R (statistical computing)
- Time resolved calibration to fix electrical field shifts



Timing sequencer control
32 channels, 16 logical connections



Stabilizer used in long term measurement (12h), jitter 130 ns reduced to 40 ns



Main User Interface, top: time distribution of intensity , bottom: spectrum of caffeine

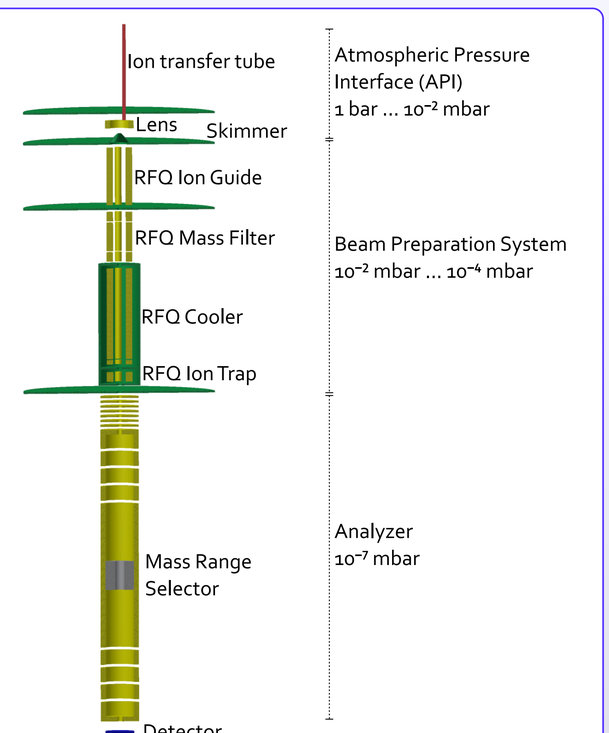
Setup



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

Performance

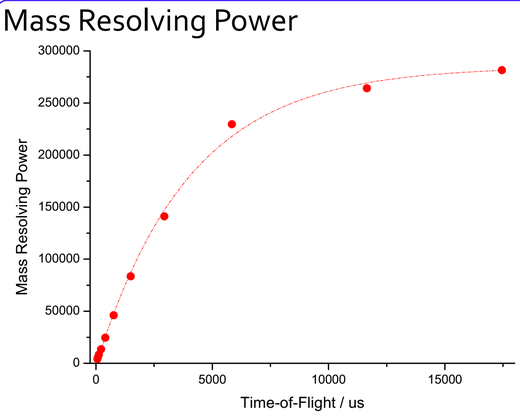
Repitition rate: 1 kHz
Atmospheric Ion Source
Mobile setup: 0.8 m³
Power consumption < 1.5 kW



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

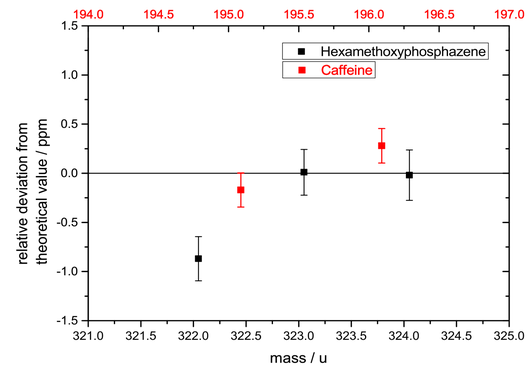
Setup Characterization

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]

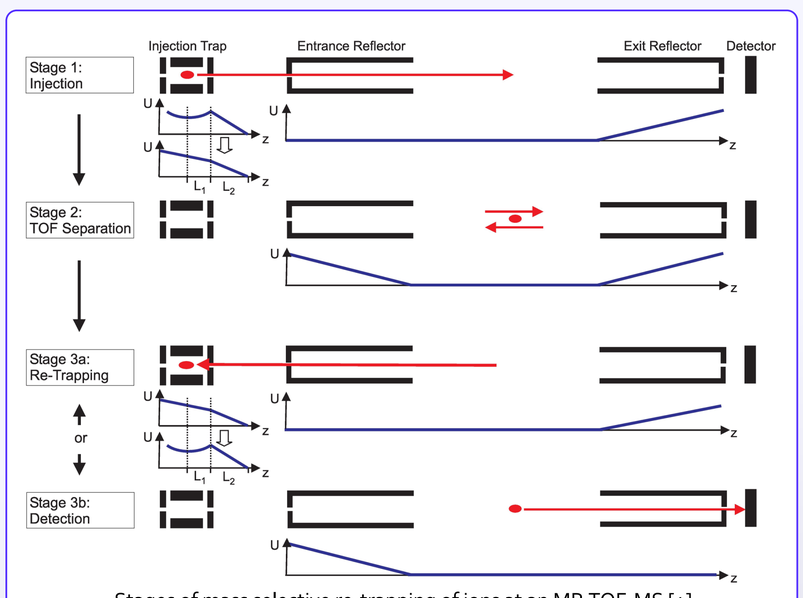
Features

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

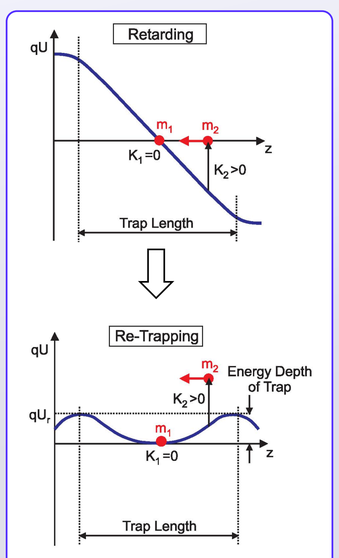
Re-Trapping

Work flow

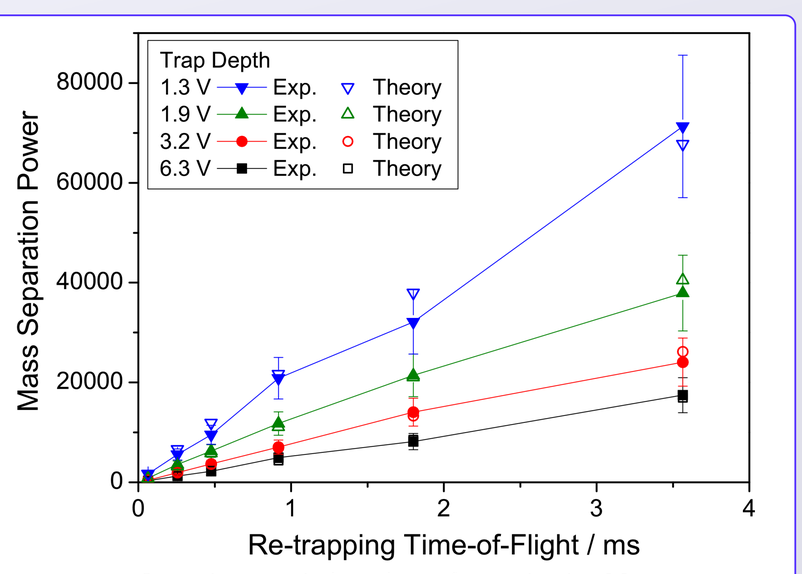
1. Ions are cooled and injected into the analyzer
2. Mirrors reflect ions to increase flight path
-> Long flight paths disperse ions in time
3a. Ions are re-trapped in the RFQ-Trap
-> CID breaks up molecules by exciting ion's macro motion
3b. Ions are injected into the analyzer again



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



Trap potentials for retrapping [3]



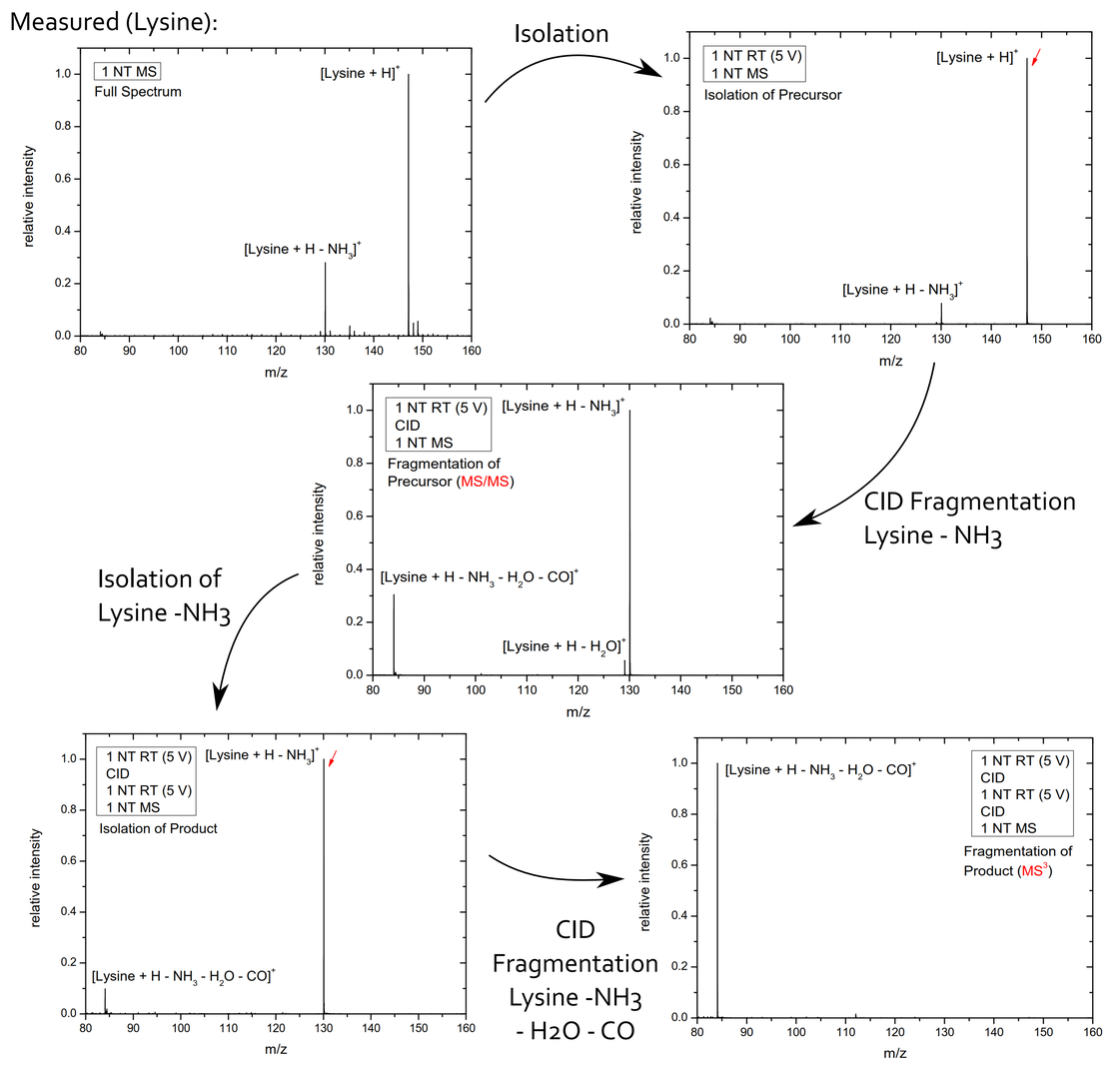
Separation power in dependence of retrapping time [3]

Features

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

MS³ 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 disspciated



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., NIMB,2013, 317 (PartB), 779-784
[2] J. Lang, PhD thesis submitted
[3] W. Lippert, PhD thesis, 2016, JLU Gießen
[4] T. Dickel et al., submitted, JASMS (2016)

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