

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 acquisition, analysis and hardware control.

Hardware control

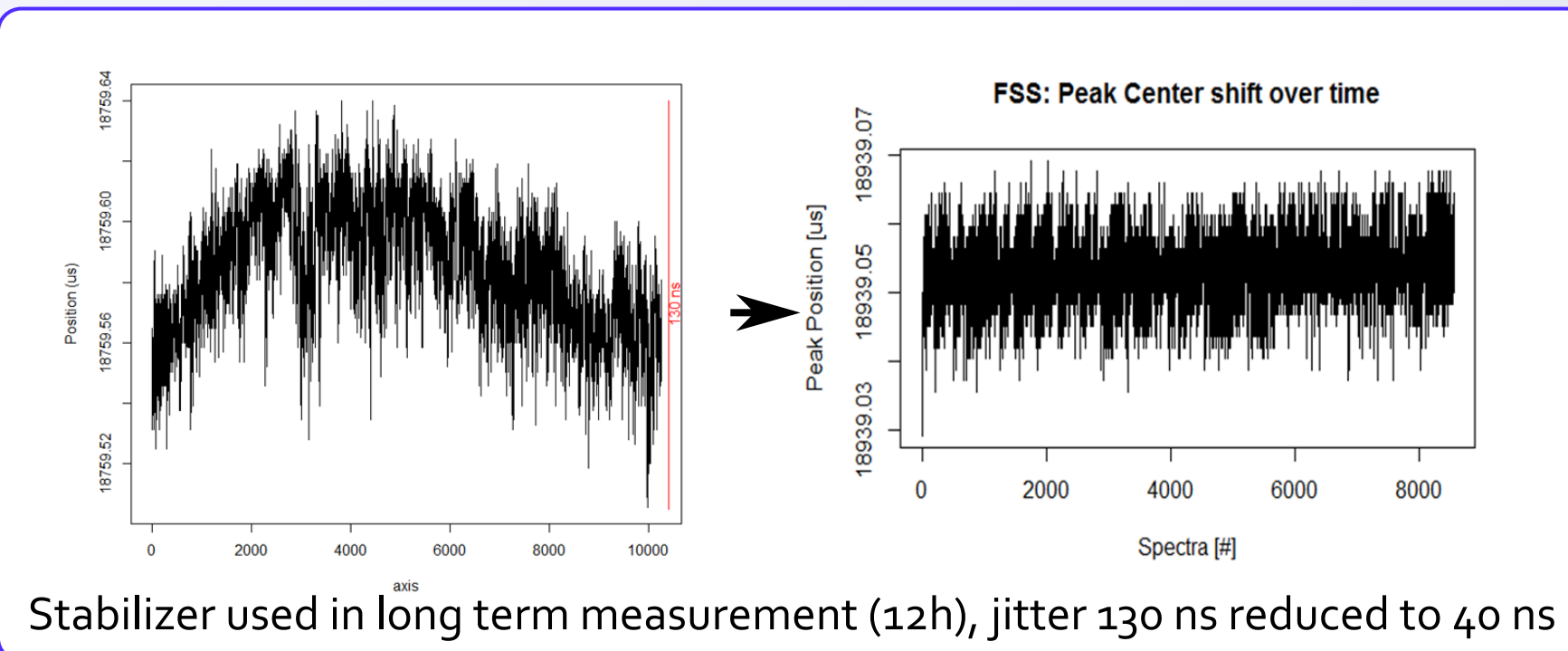
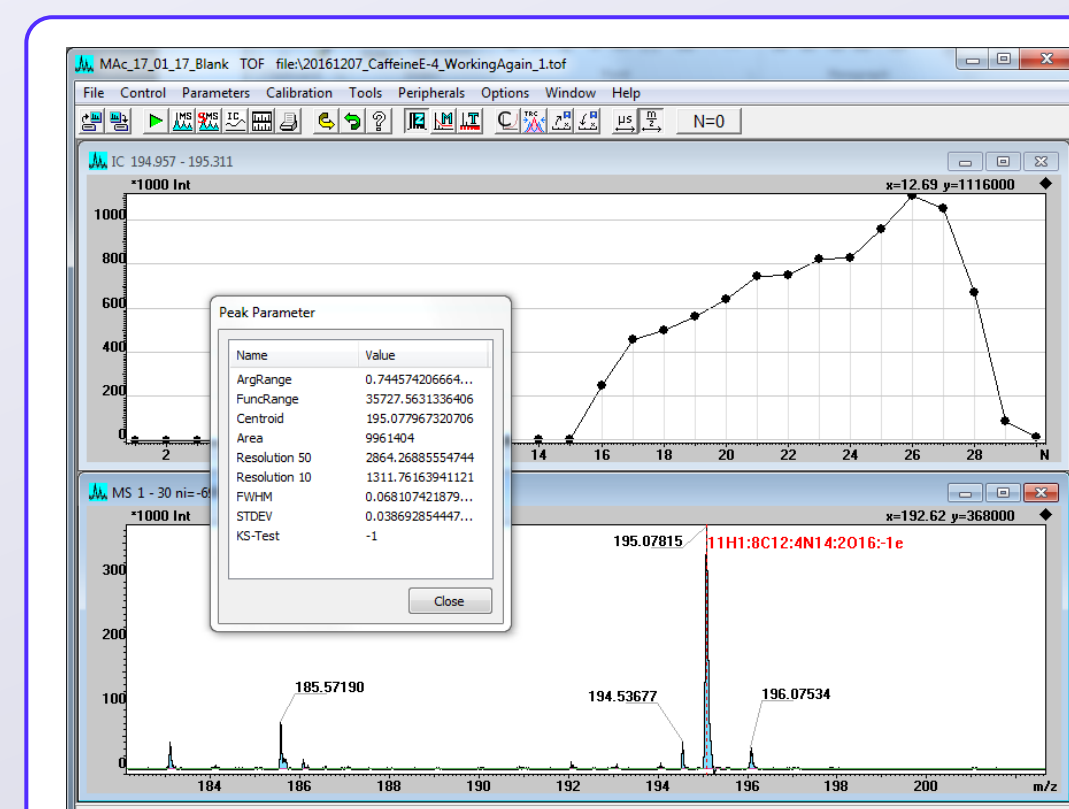
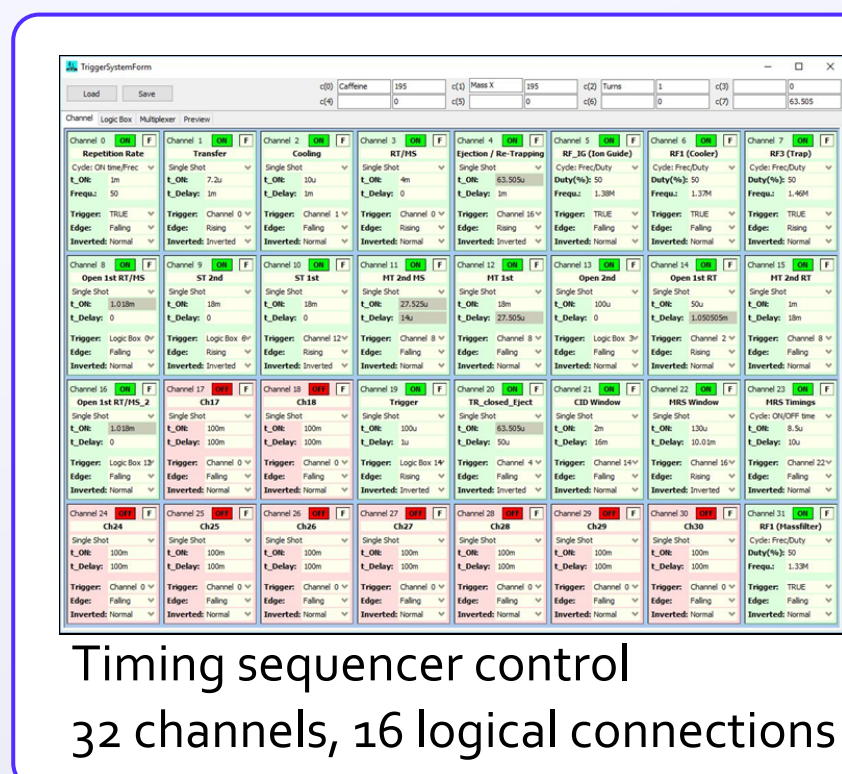
- Full control and preview of RFQ time sequencer via fpga board
- Optimizer can access applied voltages and time sequencer
- Feedback software stabilizer keep flight times stable

Data Acquisition

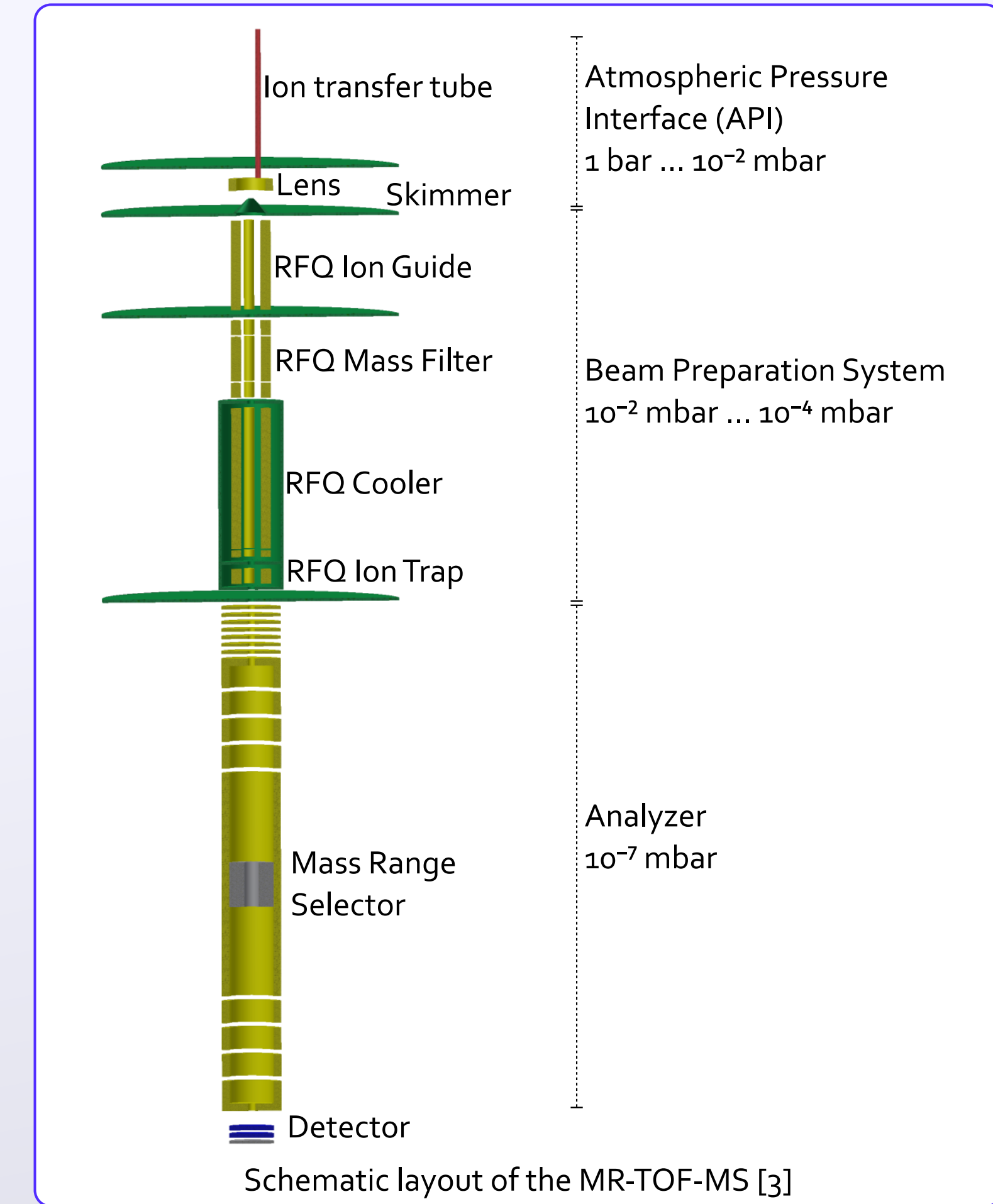
- Support of parallel ADCs/TDCs for increased dynamic range
- Enables long term measurement with auto-save feature

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



Setup

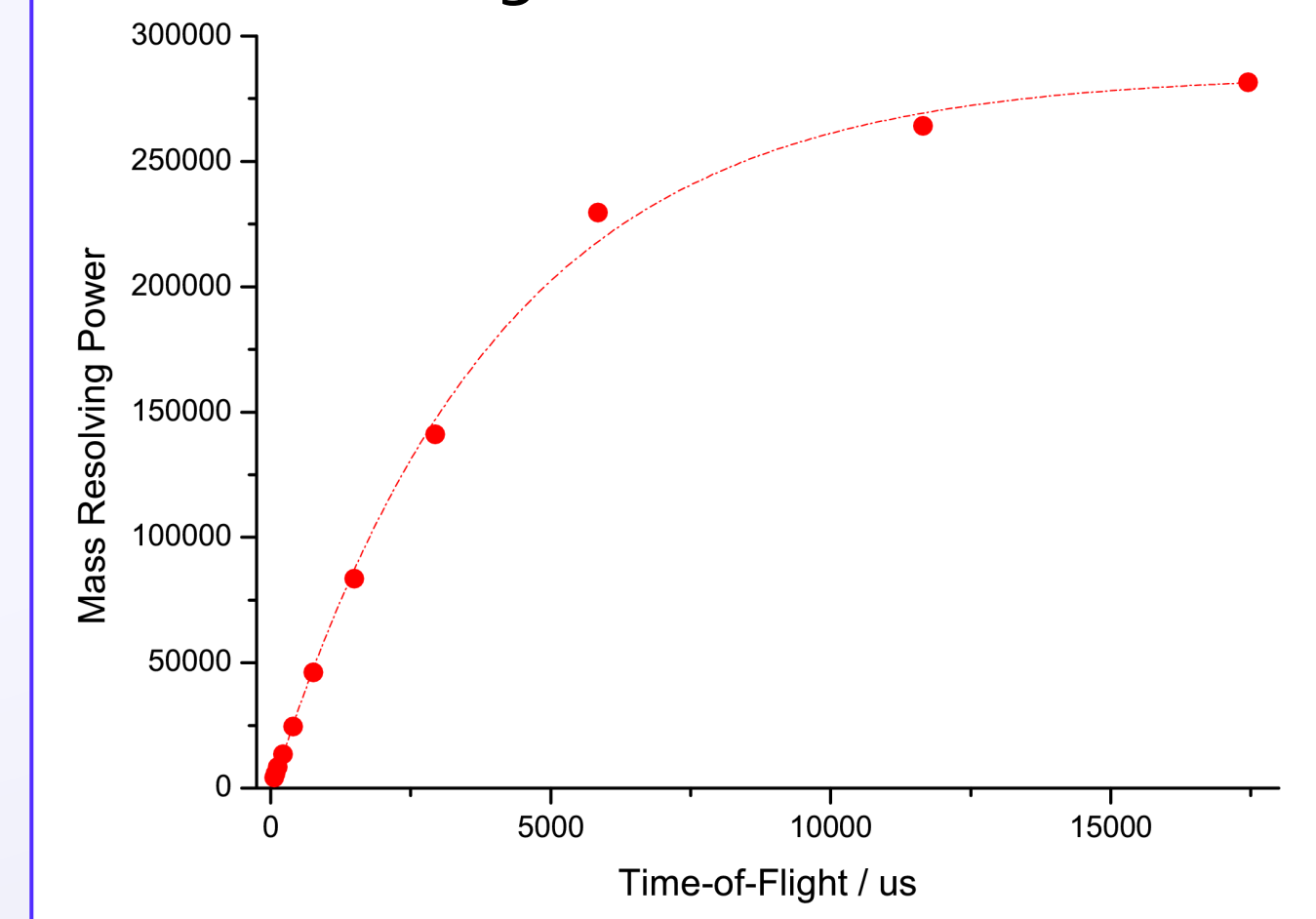


Performance

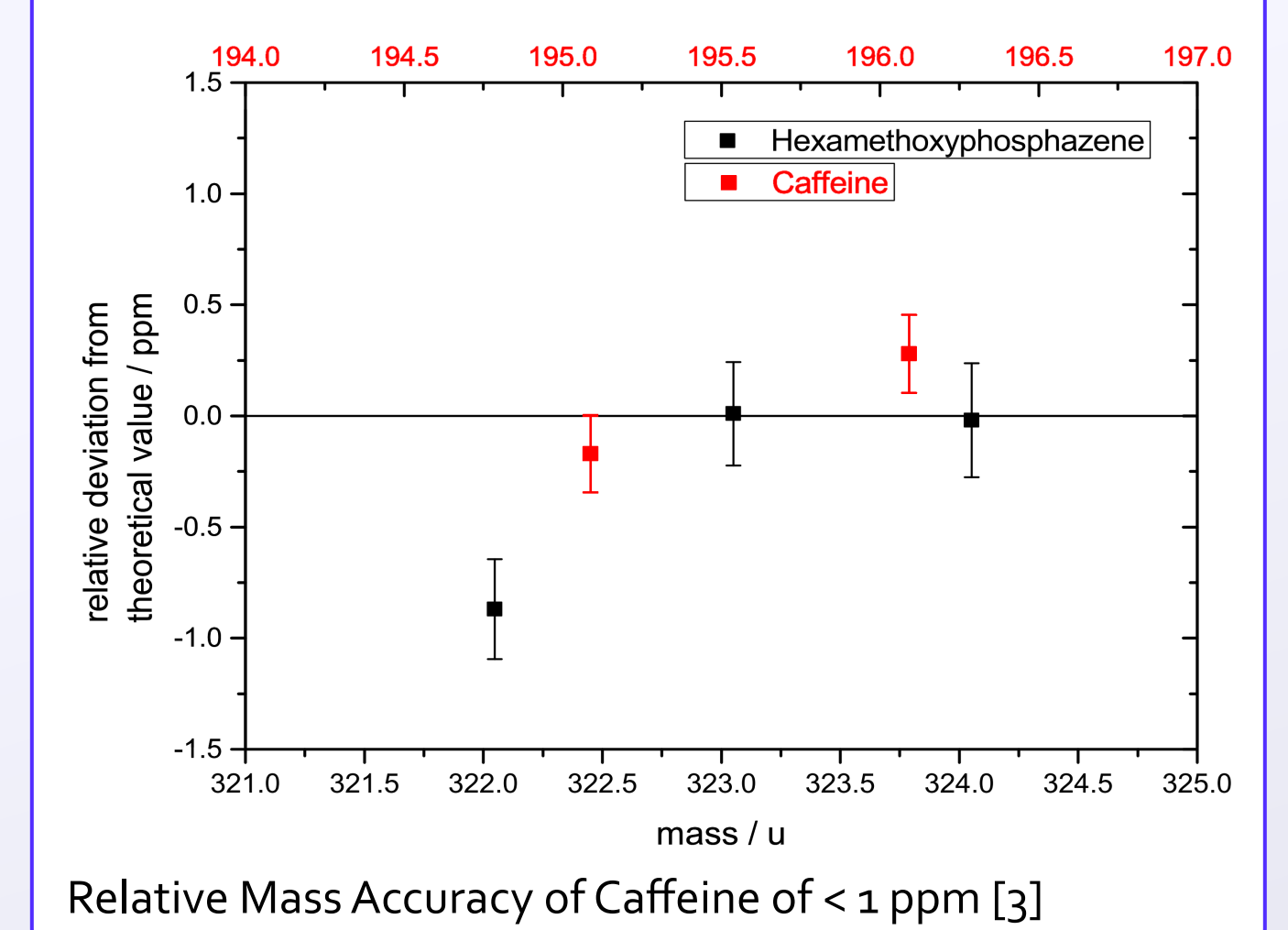
Repetition rate: 1 kHz
 Atmospheric Ion Source
 Mobile setup: 0.8 m³
 Power consumption < 1.5 kW

Setup Characterization

Mass Resolving Power



Mass Measurement Accuracy:



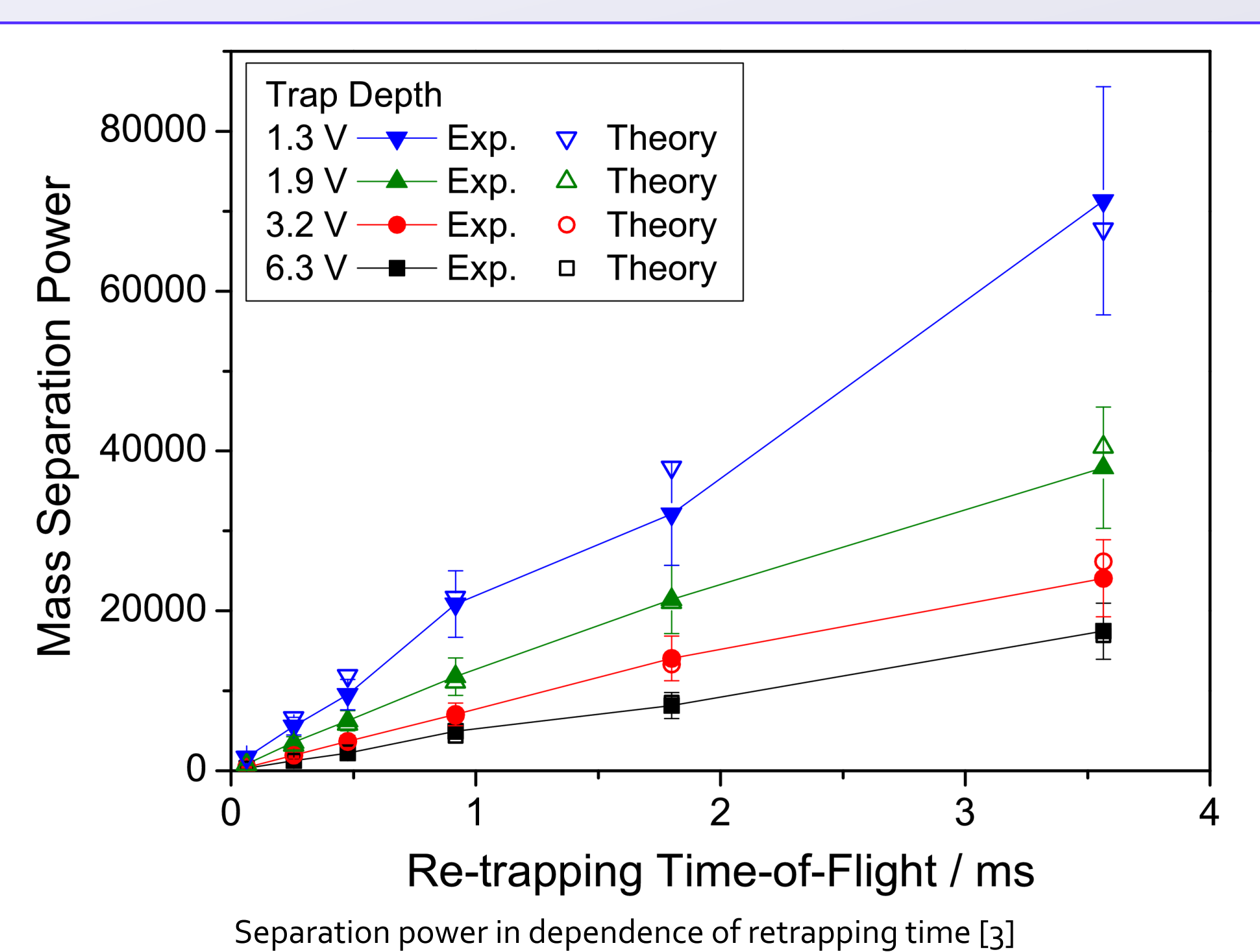
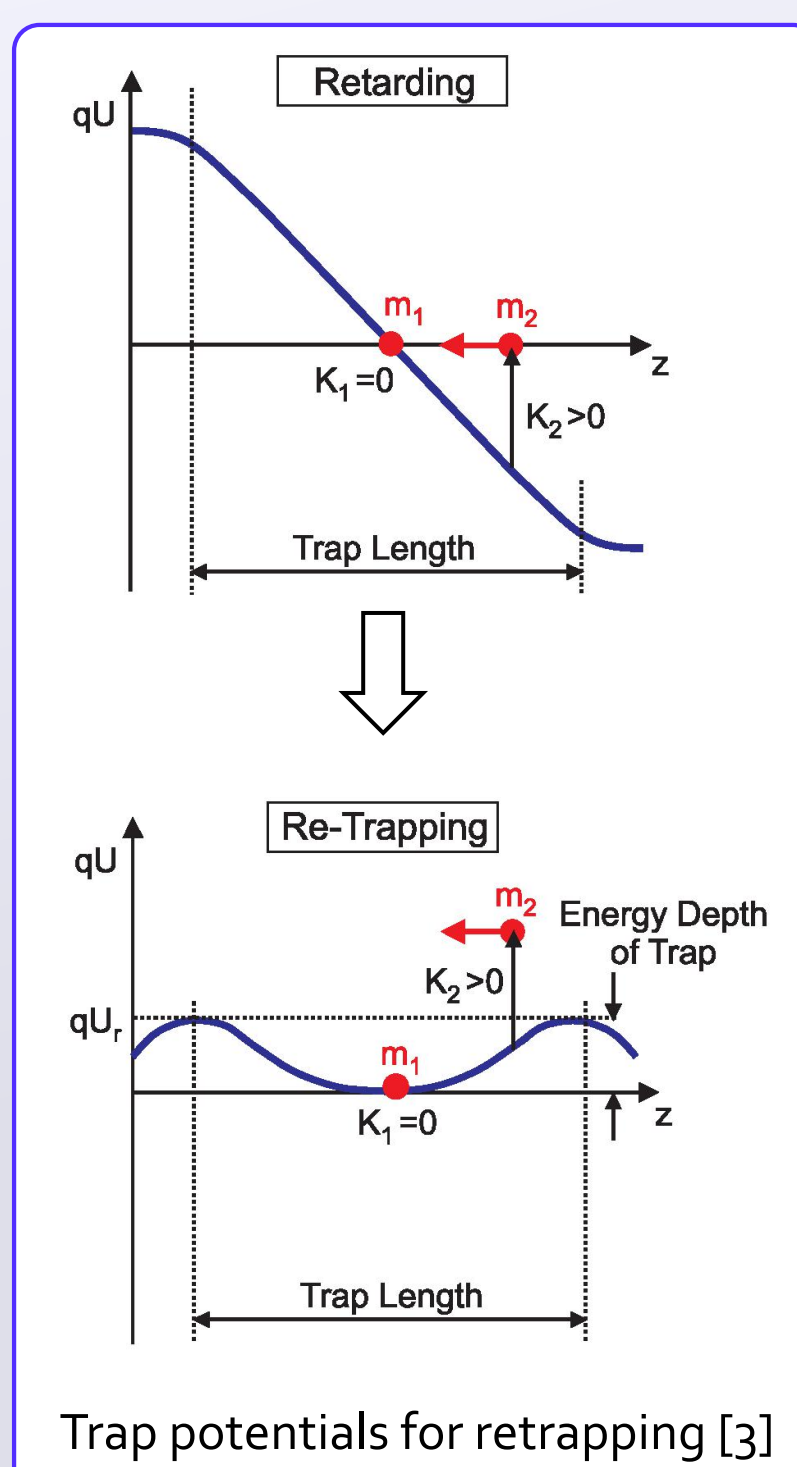
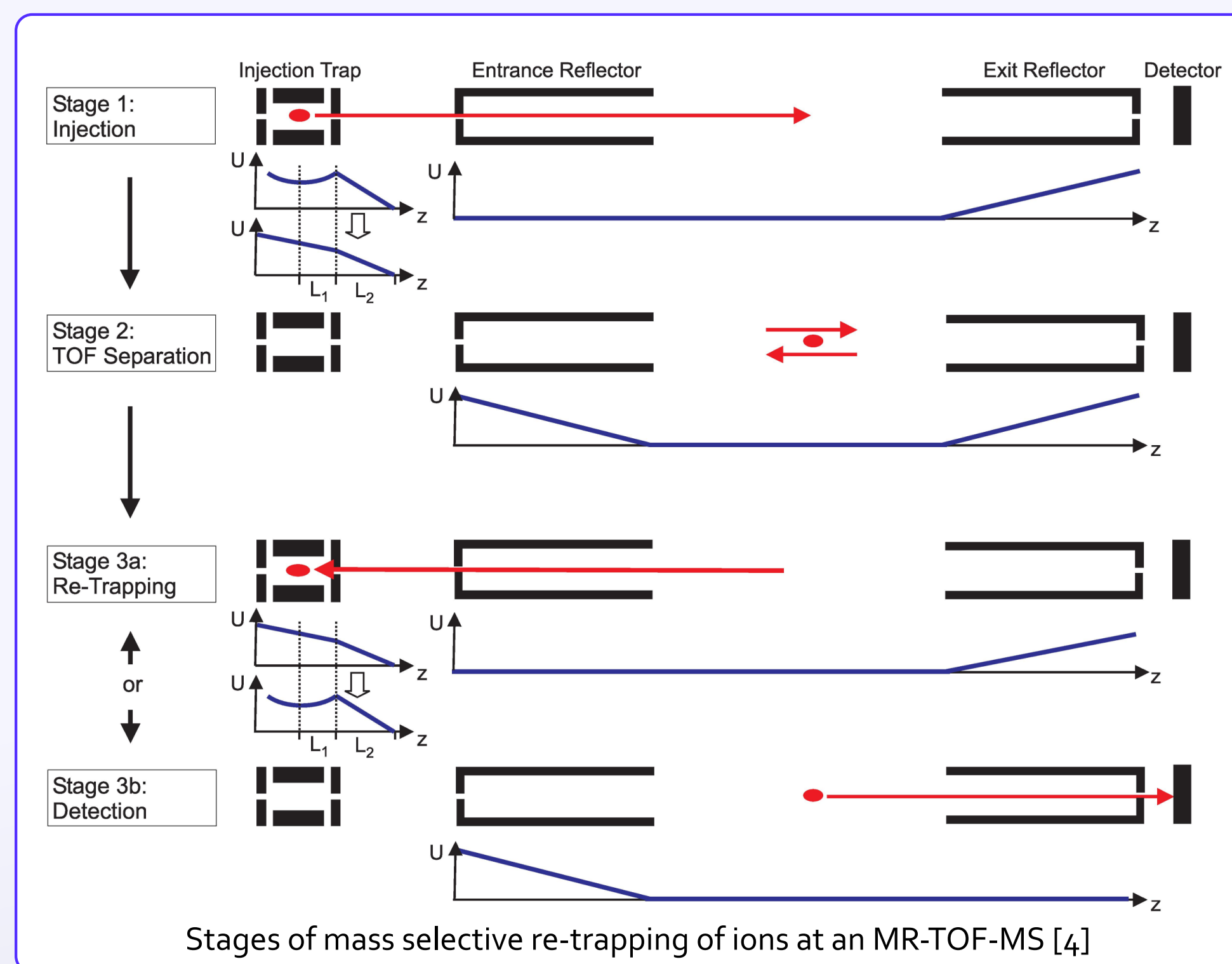
Features

- 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

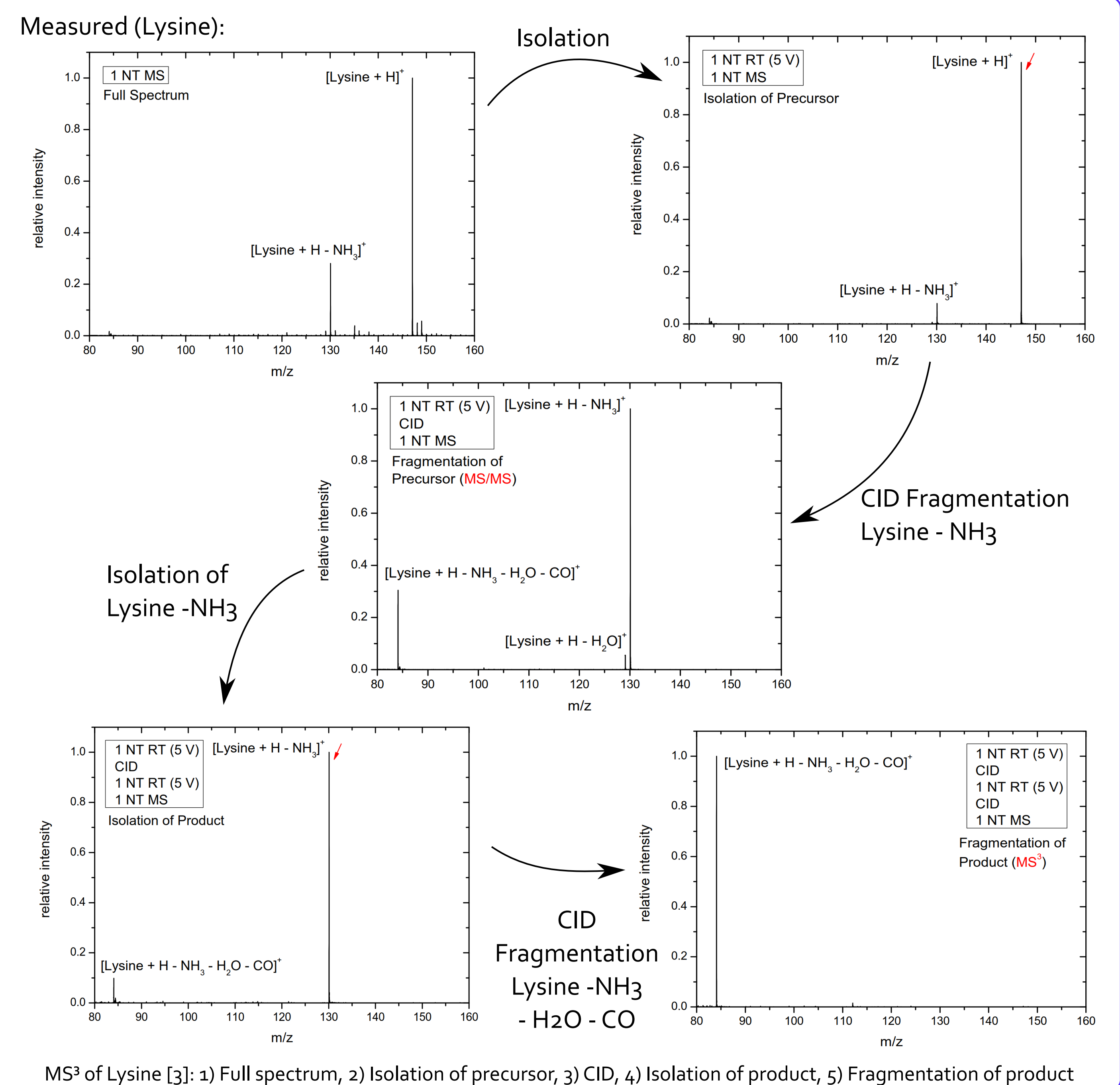


Features

- 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 - NH₃ (C₆H₁₂N₁O₂) at m = 130 u was again isolated and dissociated



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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