Accelerated Time of Flight Mass Spectrometry

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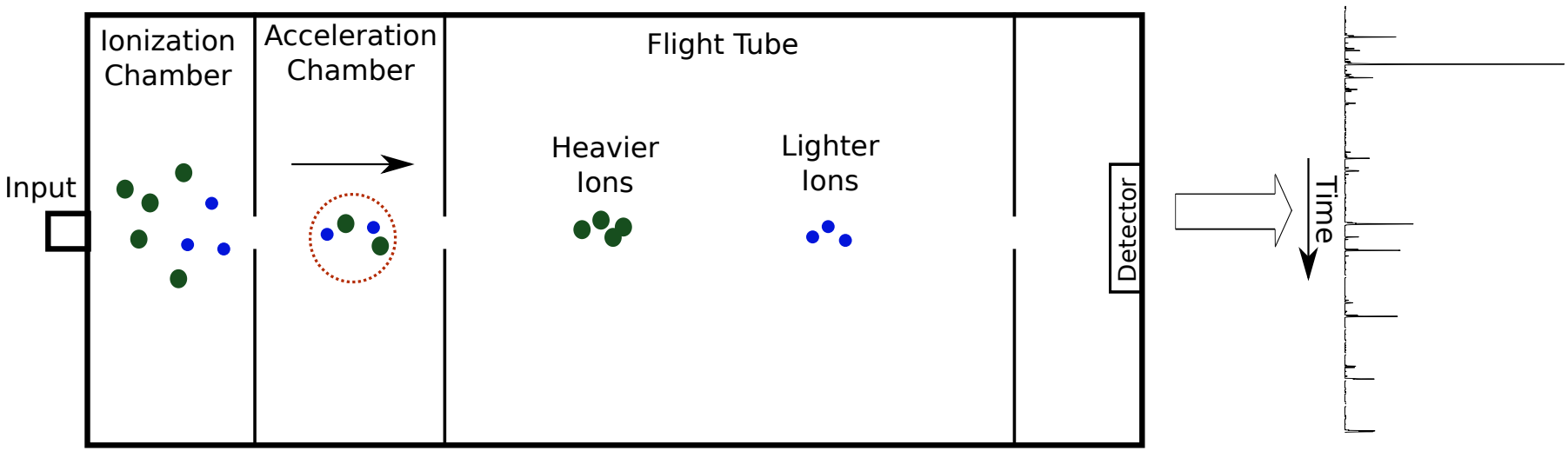
Time of flight mass spectrometry (TOFMS)

Ion **packets** are accelerated into flight tube

Impact detector at the end of the path

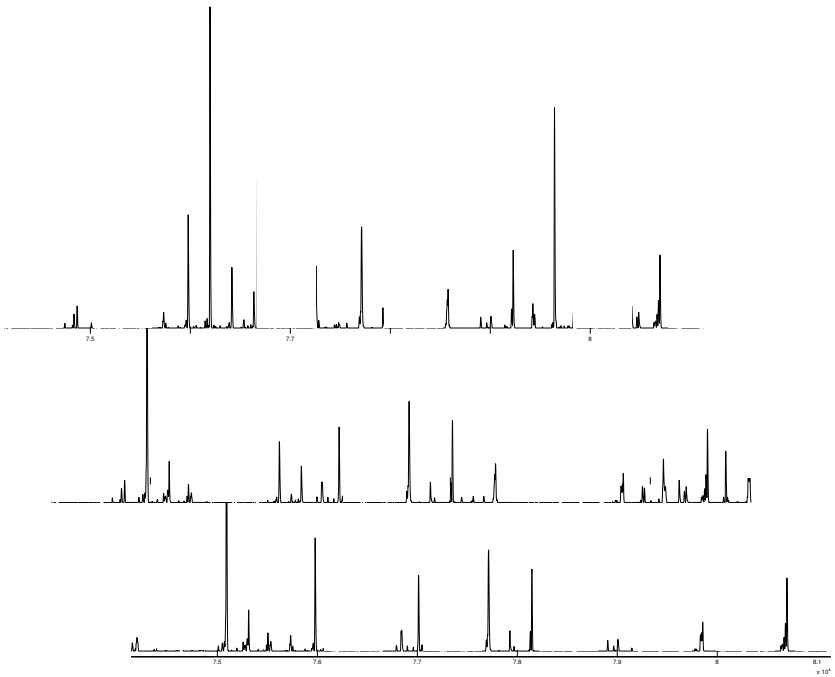
Observed signal $\rightarrow$ one **scan** of $\sqrt{m/z}$ spectrum

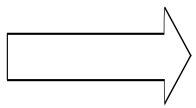


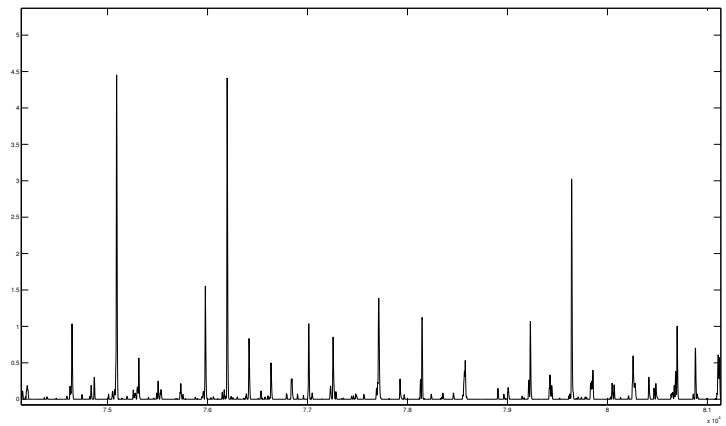
Simple depiction of a TOFMS
(Figure courtesy of KORE Technology)

Obtaining a clean spectrum

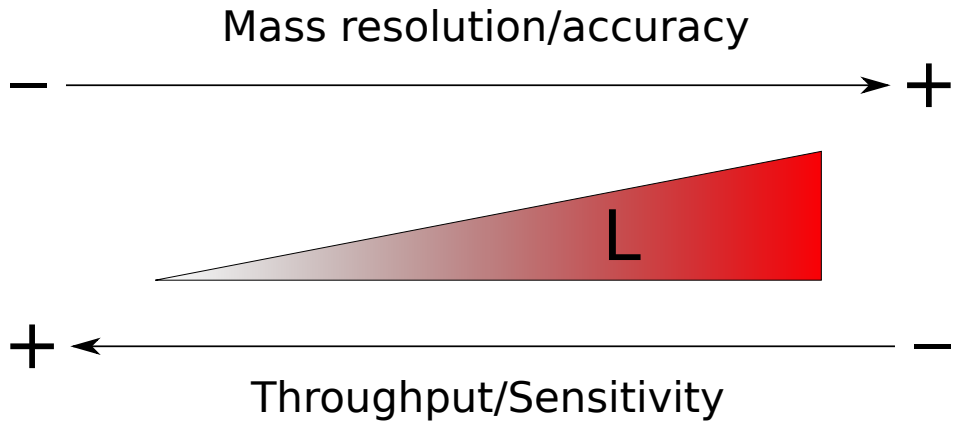
One scan is too noisy $\rightarrow$ $N \approx$ 100's-1000's scans are required







The trade off between mass accuracy/resolution and sensitivity/throughput



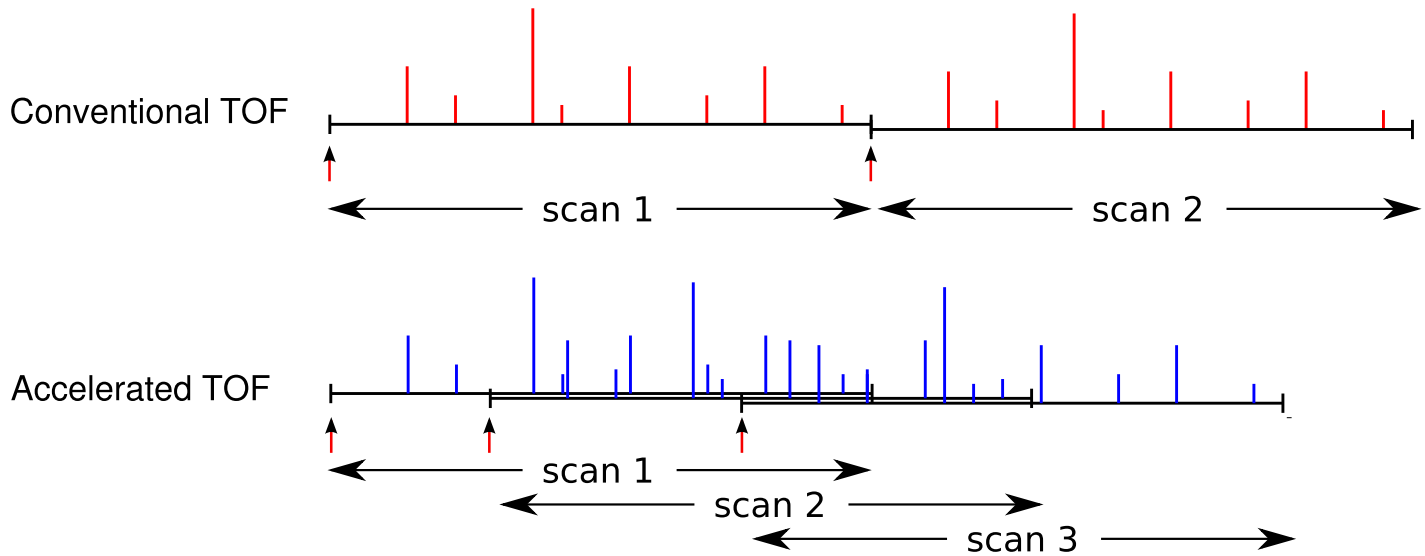
L: Length of the flight tube

Accelerated TOF (ATOF)

- TOF $\rightarrow$ Have to collect many scans
- Each scan is a very sparse signal

Idea

Increase the repetition rate and allow the subsequent scans to overlap



Challenge

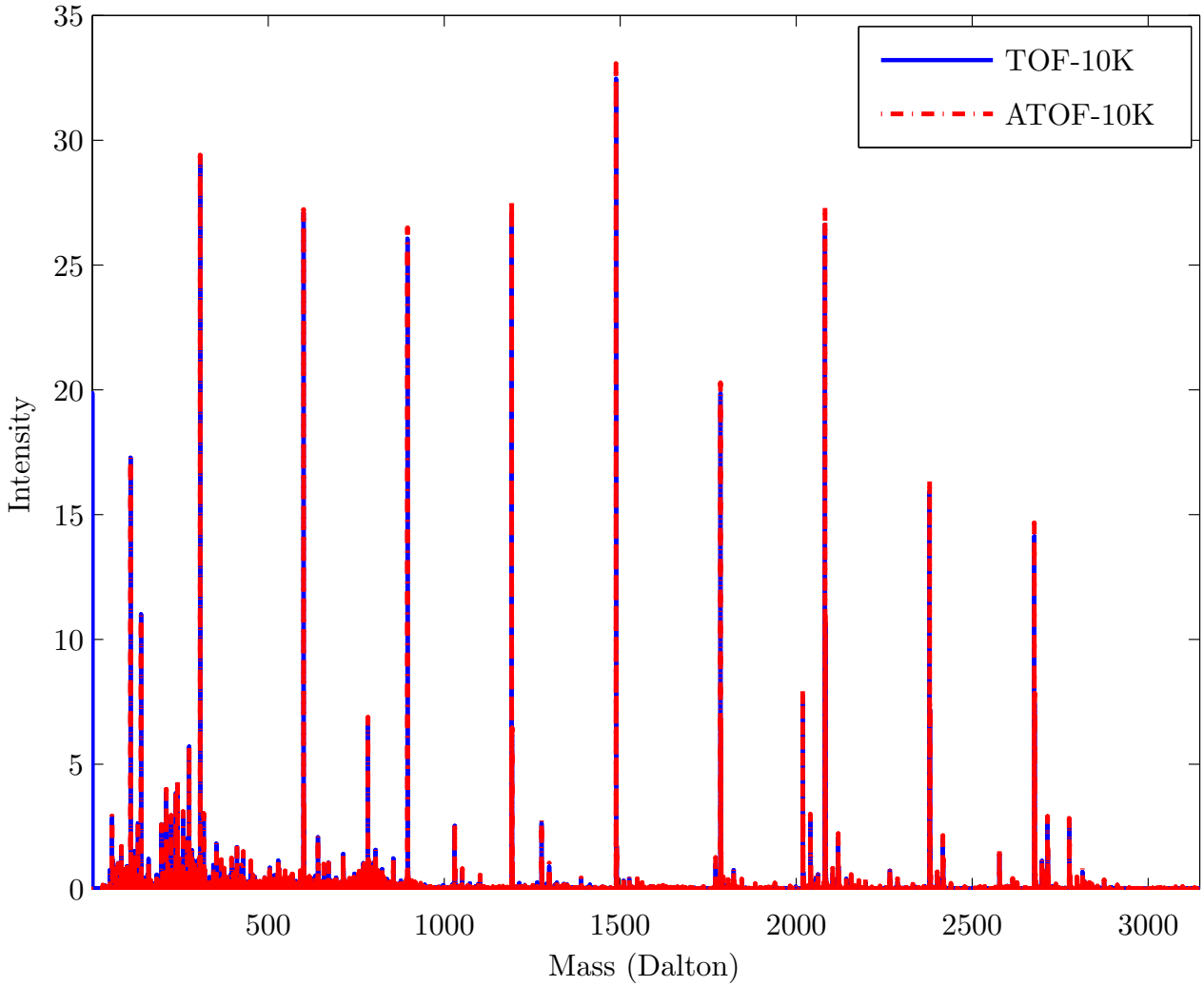
Recover spectrum from overlapped scans

Accelerated TOF Hardware

ATOF requires little alteration to the existing hardware

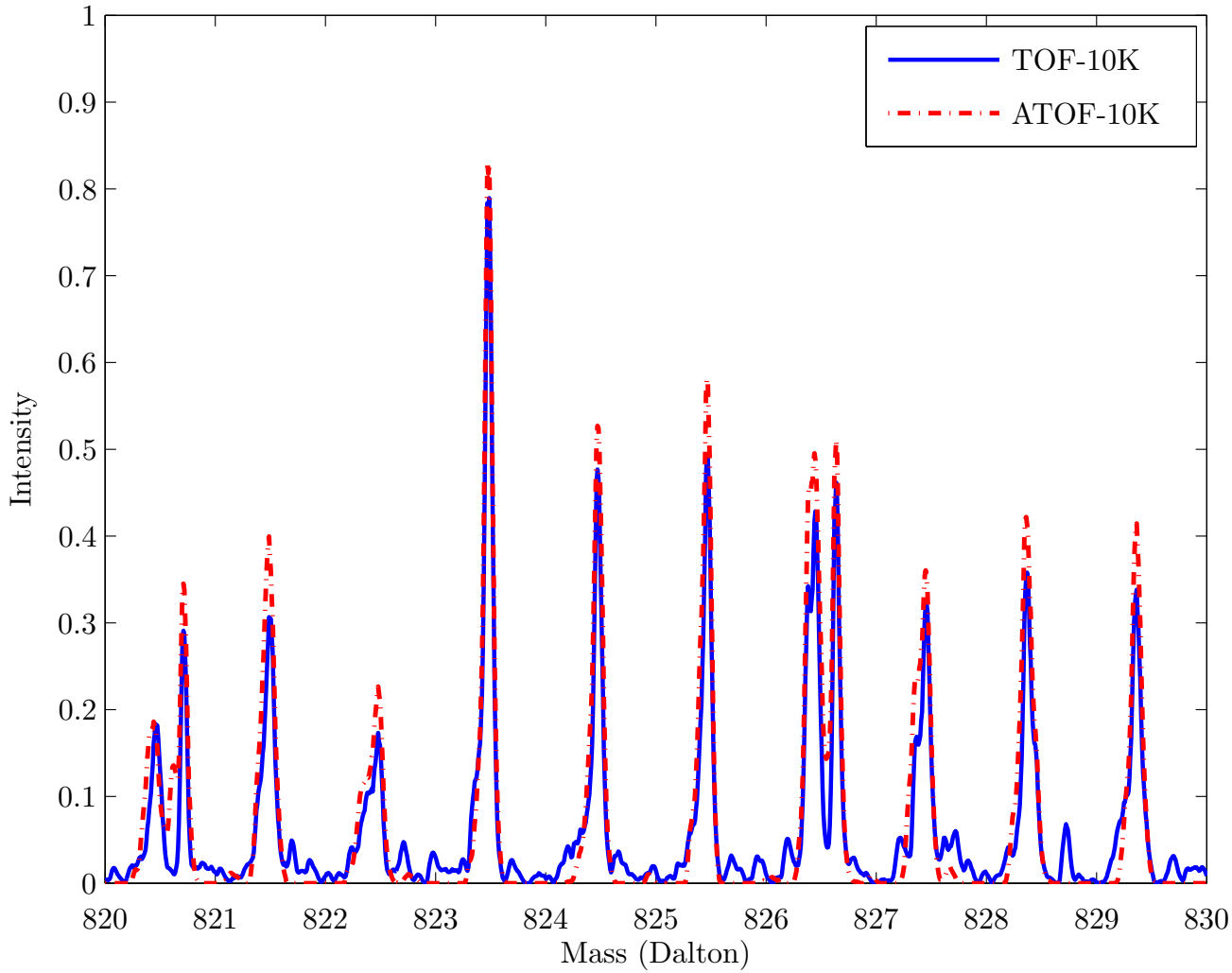
- → Ion acceleration unit to *fire* at irregular pseudo-random intervals
- → More elaborate post-processing computation unit

Sample spectrum for conventional TOF and ATOF



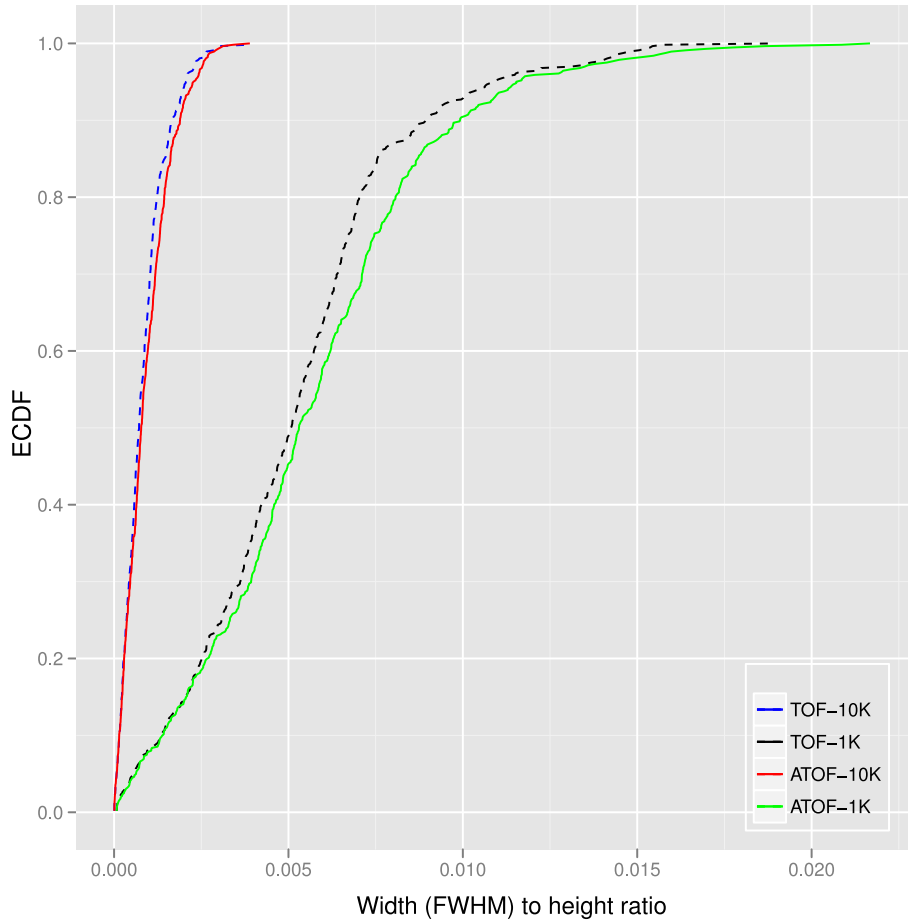
Acceleration factor = 10

Sample spectrum for conventional TOF and ATOF



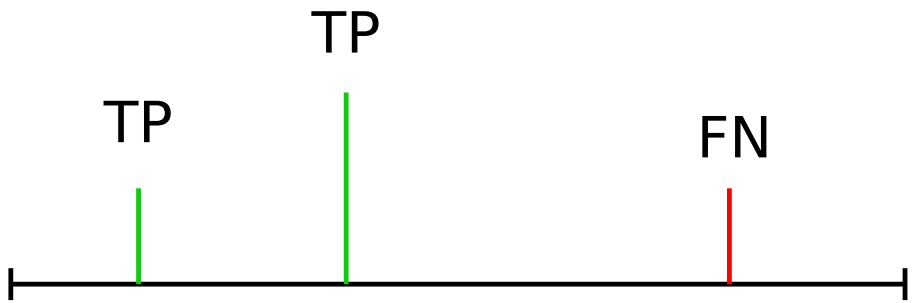
Acceleration factor = 10

Evaluating ATOF: Peak shapes



ATOF does not change or broaden the peak shapes

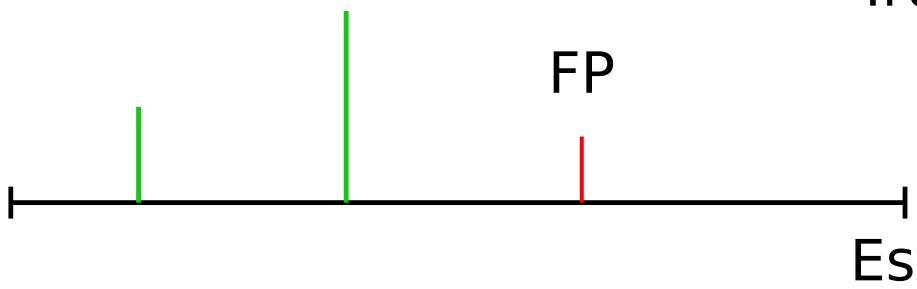
Evaluating ATOF: Performance criteria



True positive (TP)

False positive (FP)

False negative (FN)

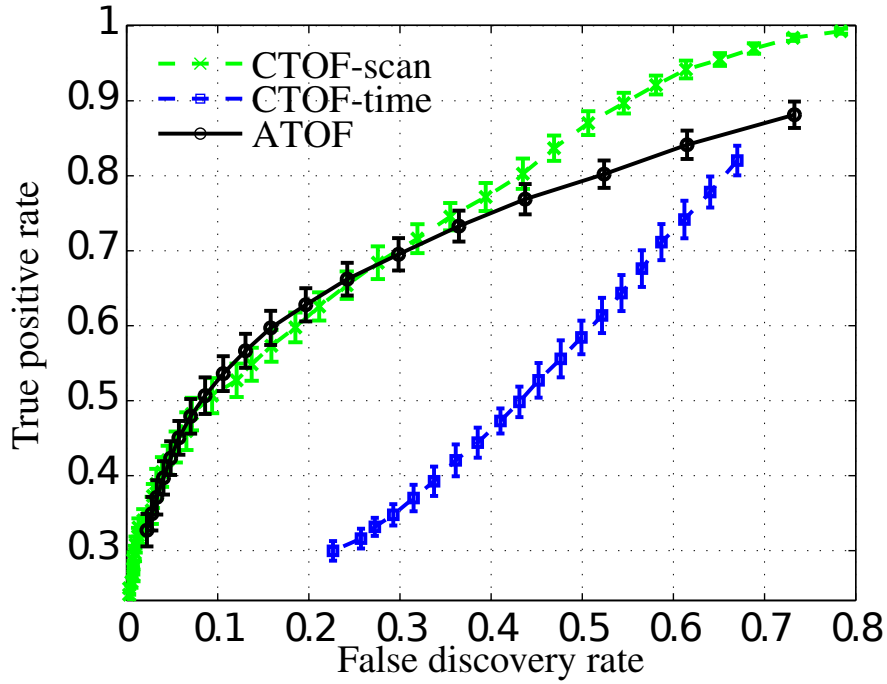


True positive rate (TPR) = TP/(TP+FN)

False negative rate (FNR) = FN/(TP+FN) = 1-TPR

False discovery rate (FDR) = FP/(FP+TP)

ATOF vs CTOF



CTOF-scan: Conventiaonl TOF with same number of scans as ATOF

CTOF-time: Conventional TOF with same amount of acquisition time as ATOF

ATOF Summary

- ♢ Simple modification of the conventional TOF with minimal change in hardware

Our contribution:

- ♢ An efficient algorithm for *online* reconstruction of spectrum
- ♢ Can speed up a conventional TOF instrument by an order of magnitude