- ToF-CIMS, IMS-TOF, and FIGAERO
- DAQ5
- Event Trigger Mode
- ePToF

Friday - "CIMS and ToF-AMS DAQ updates"
Sunday - "Overview: Event Trigger and ePTOF"

Aerodyne ToF-CIMS

- **Over 40 instruments**
  - US, Europe, Asia
  - Lab, ground sites, aircraft, RVs
- **Collaborative user community – similar to AMS.** 60 attendees at this year's users meeting. Next meeting will be in Finland in Spring 2016.
- **"Tofware" Advanced analysis software –** paradigm mimics Squirrel. Led by H. Stark and M. Cubison.
- **Diverse applications**
  - **Ion chemistry ->** Different classes of compounds
  - **FIGAERO Inlet ->** Aerosol and gas-phase sampling

ToF-CIMS Hardware

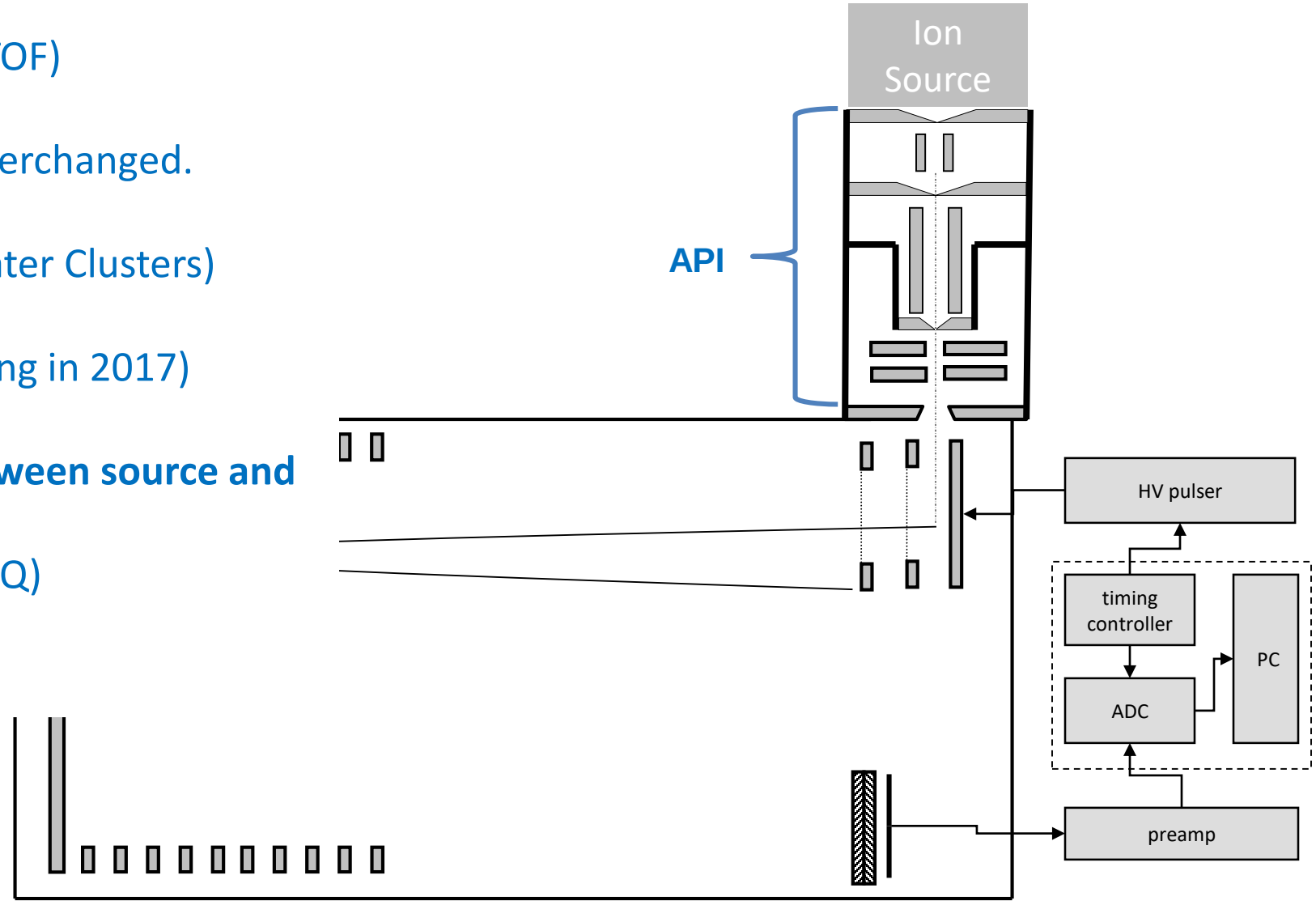
Same TOF as AMS (CTOF, HTOF, or LTOF)

High pressure ion sources. Easily interchanged.

- **"APi" natural ions**
- **Po or x-ray IMR** (Acetate, I-, Water Clusters)
- **Nitrate** (aka, CI-APi)
- **EESI** (As presented by PSI, coming in 2017)

3 stages of differential pumping between source and TOF

- 2 RF-only quadrupoles (SSQ, BSQ)
- Focusing lenses



LTOF and HTOF Versions

1.5 m

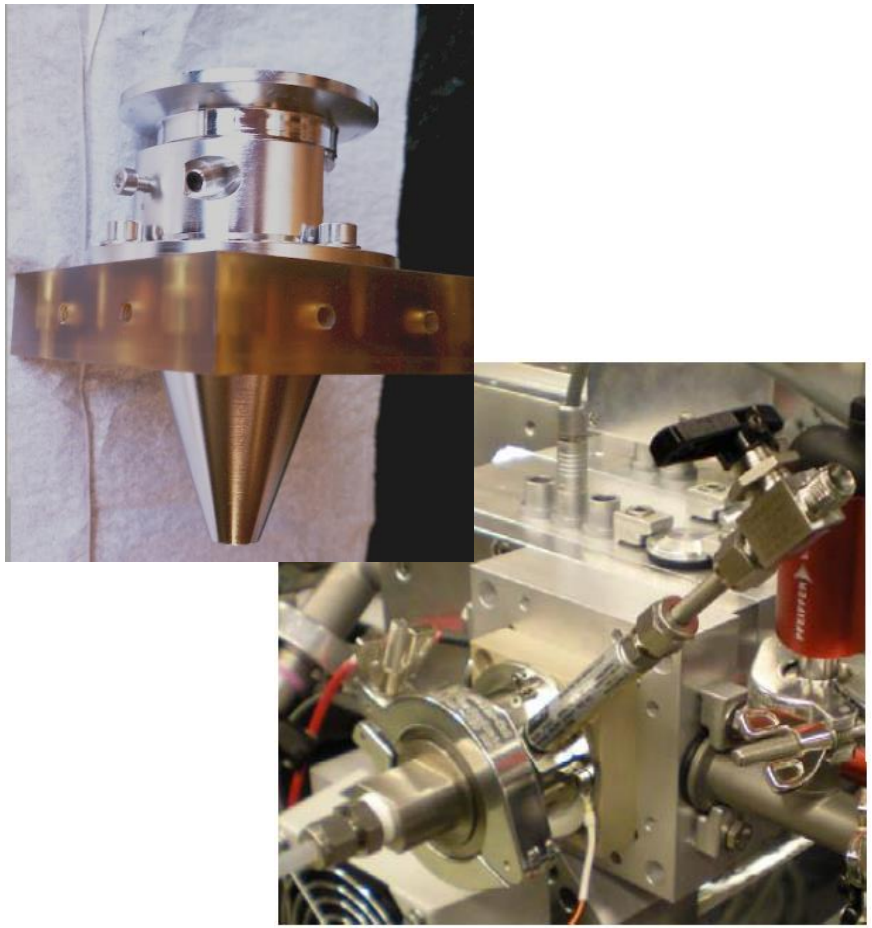
0.8 m

LToF-CIMS

HToF-CIMS

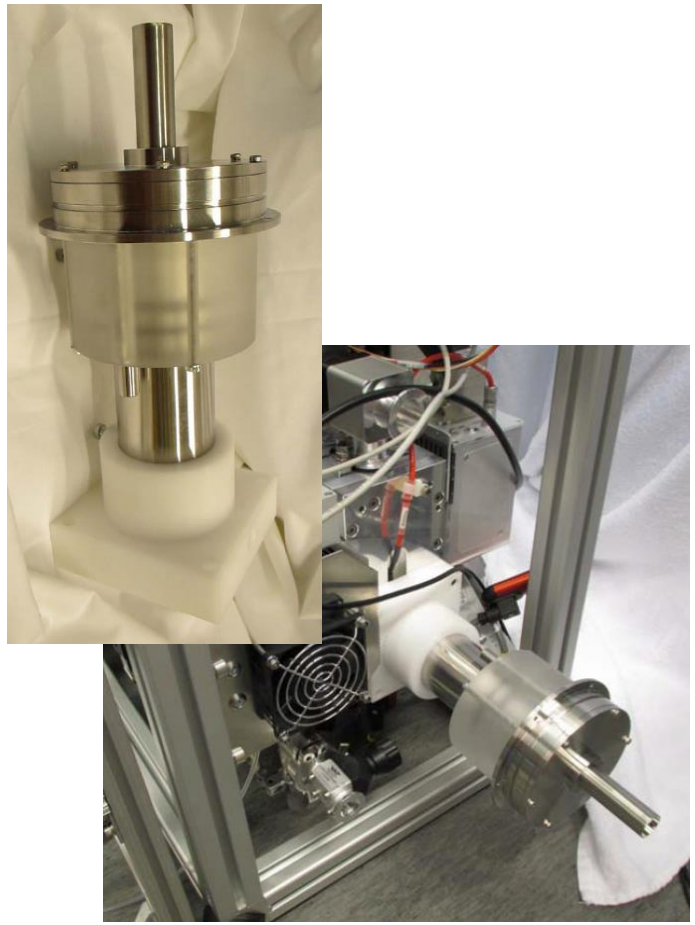
LToF-CIMS was released in 2016

- **Size:** Same footprint, ~2x height of HToF-CIMS
- **Sensitivity:** Approximately equal to HToF-CIMS
- **Resolving Power:** 2x the HToF-CIMS, approx. 10 000 and 5 000
  - New acquisition mode (currently being evaluated) that increases R of LToF-CIMS 20 to 30%



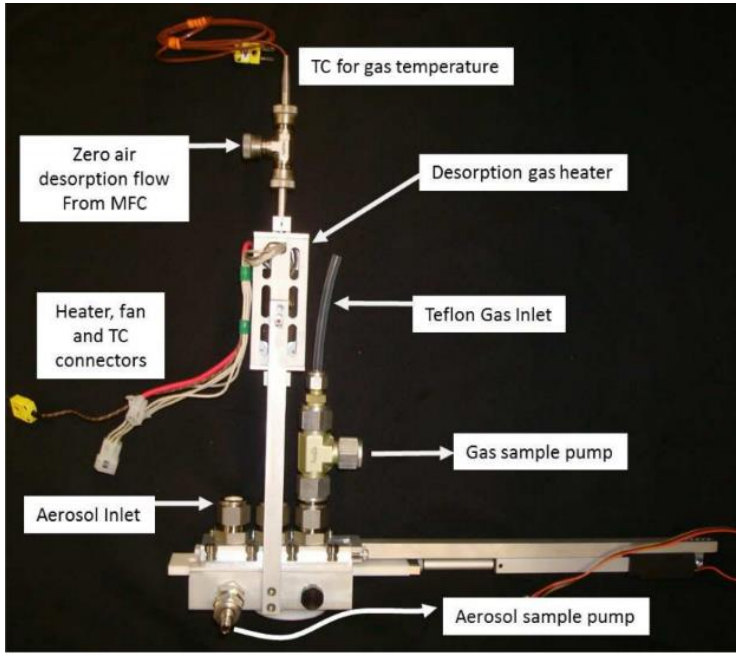
IMR

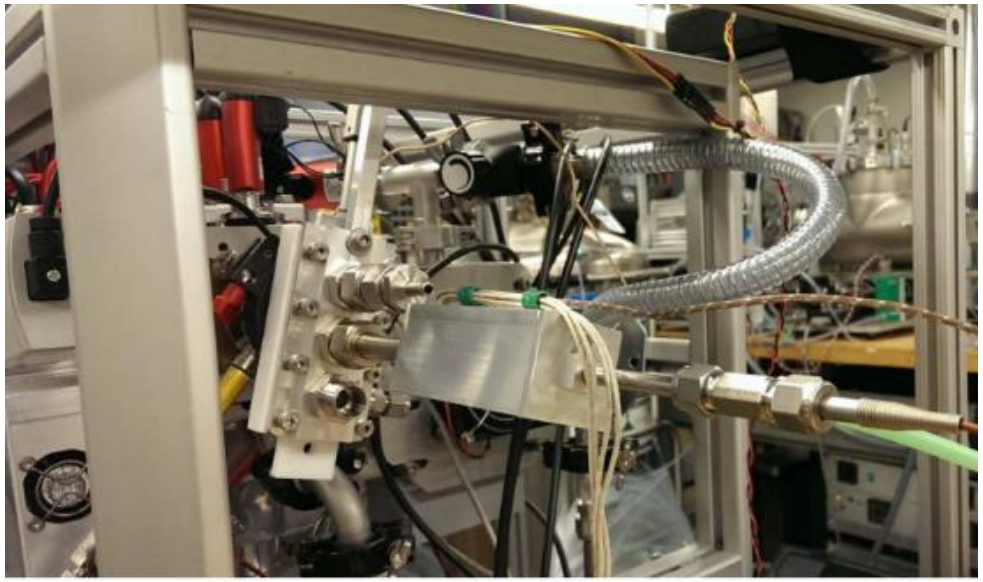
- 50 - 500 mbar
- Flow Tube
- Po-210 or X-ray ionizer
- Acetate, H30(H2O)n, I-, …
- Compatible with FIGAERO



Nitrate

- 1000 mbar
- Drift Tube
- X-ray ionizer
- Nitrate
- Not compatible with FIGAERO





Filter Inlet for Gas and Aerosol

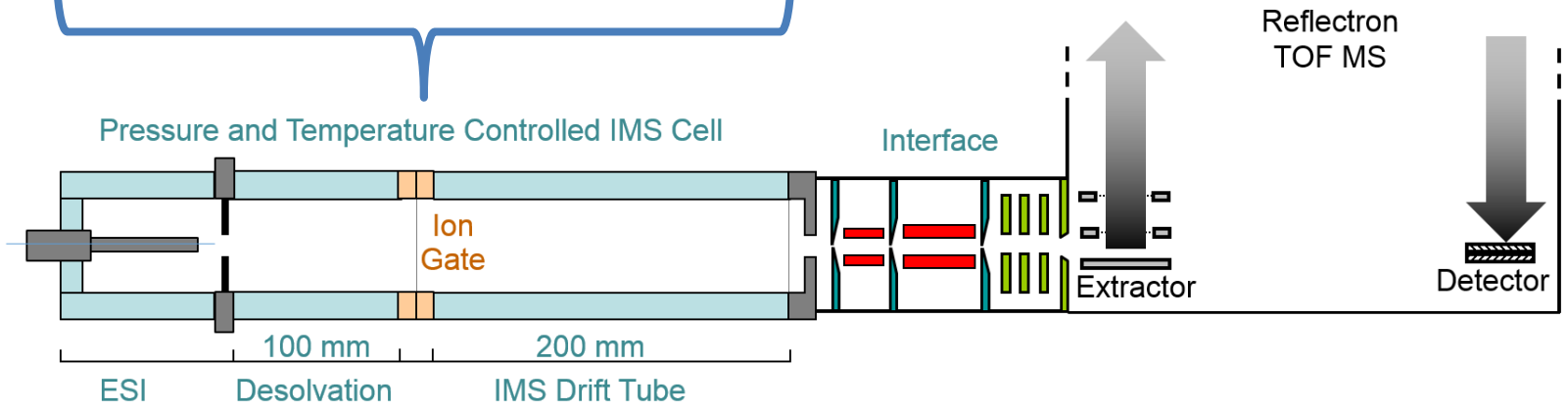
- Mounts to face of IMR, replaces standard gas-phase inlet
- Parallel gas and aerosol inlets oriented into IMR
- Alternate gas / aerosol sampling by movement of linear actuator
  - *Step 1* Gas sampled into IMR, while aerosol collected on filters
  - *Step 2* Collected aerosol thermally desorbed into IMR, with no sampling of gas phase
- Sampling cycle programmatically controlled by EyeON electronics and software

IMS-TOF

- Ion mobility spectrometer (IMS) coupled to an API-TOF
- IMS separates ions by collision cross section (CCS)
  - 2D separation increases peak capacity and improved identification
  - Resolve isomers – not possible with MS
- Optional collision induced dissociation (CID) between IMS and MS

Atmospheric-pressure, drift-tube IMS
Highest resolution of any commercial IMS

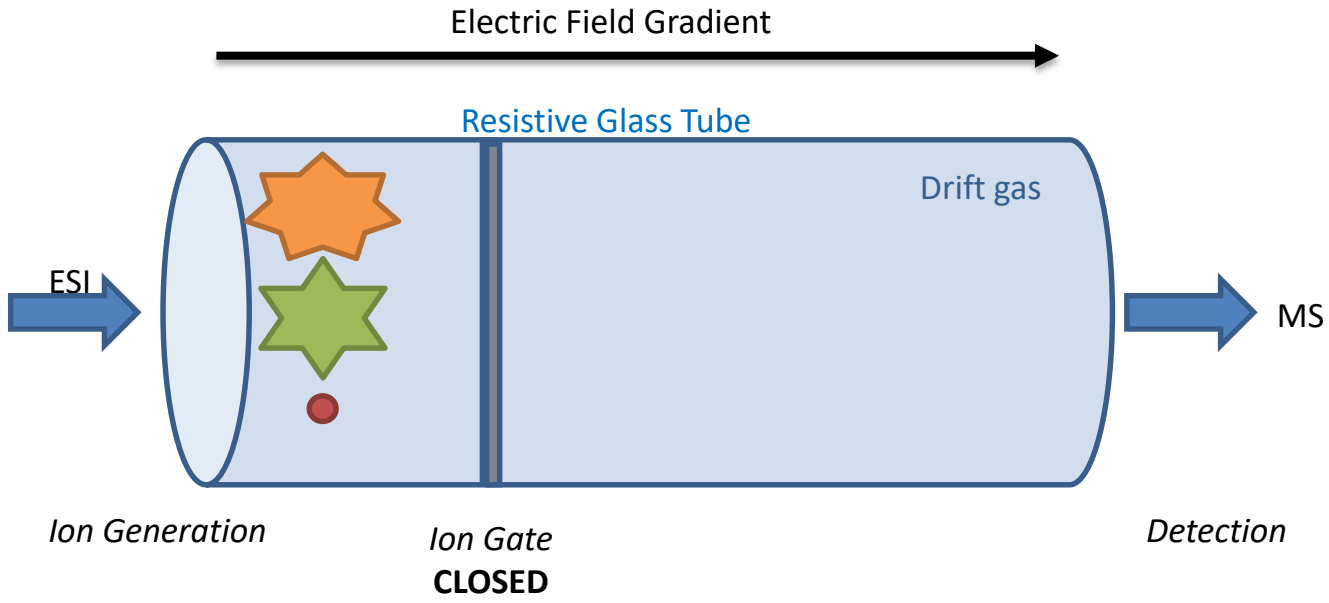
Ionization
Nitrate CI
ESI



HTOF or LTOF

How does IMS work?

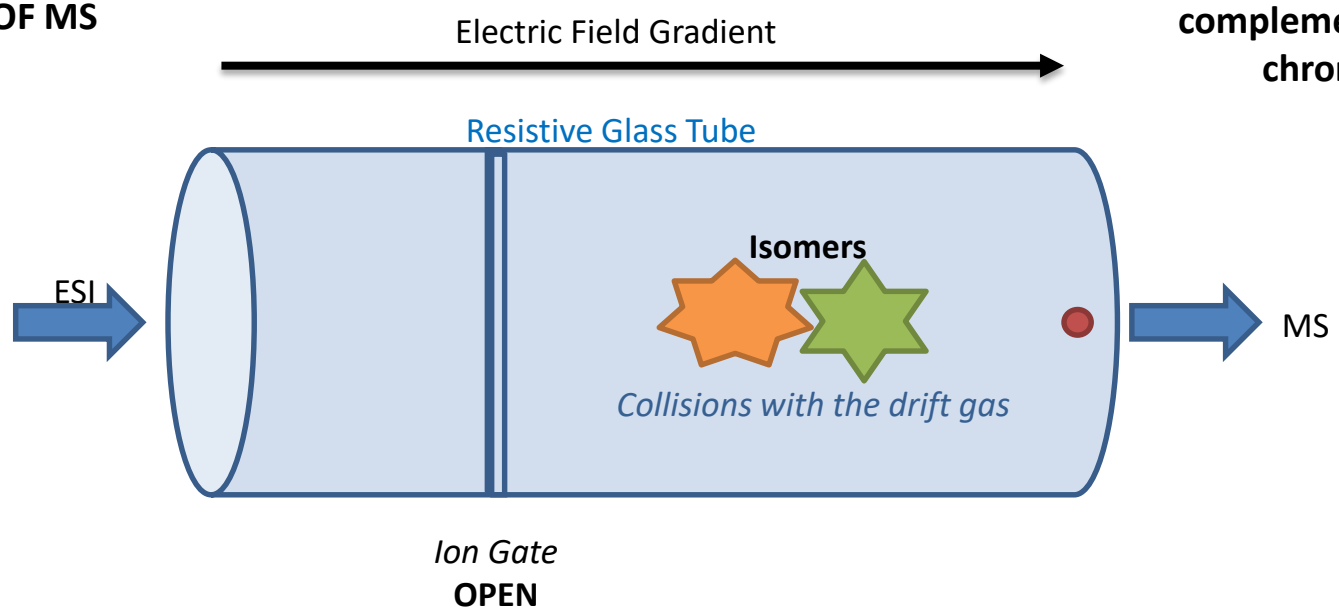
1. Ions are generated but stopped by the ion gate



Slide from M Groesl, Tofwerk

How does IMS work?

2. Ion gate is opened, ions are separated in the drift tube and detected by TOF MS



Collision cross section σ depends on size, shape, charge and mass → complementary to MS and chromatography

$$\sigma = \frac{3}{16}\left(\frac{2\pi}{\mu k T}\right)^{1/2}\frac{QE}{v_d n}$$

σ = integrated collision cross section

μ = reduced mass of the analyte and the drift gas

k = Boltzmann's constant

T = temperature

Q = ion charge

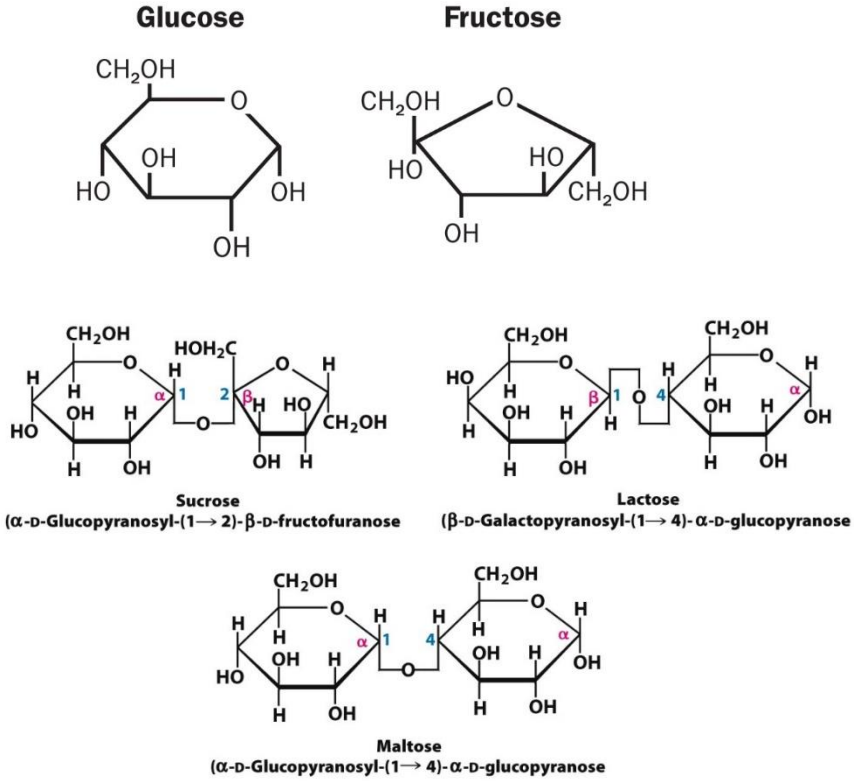
E = electric field

v_d = drift velocity

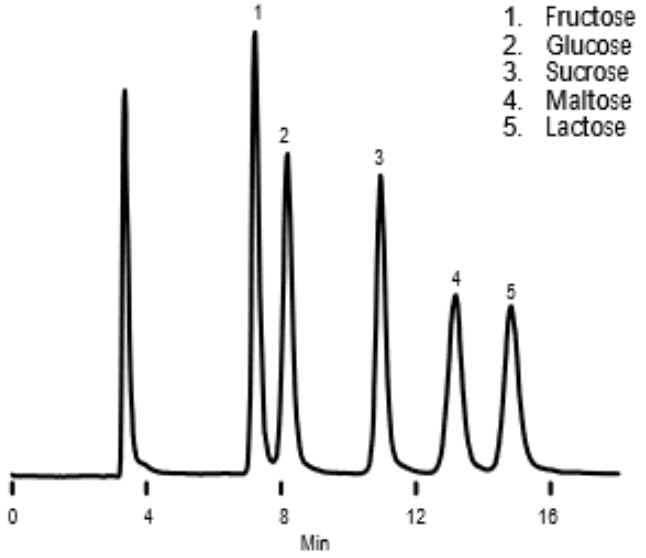
n = neutral gas number density

Slide from M Groesl, Tofwerk

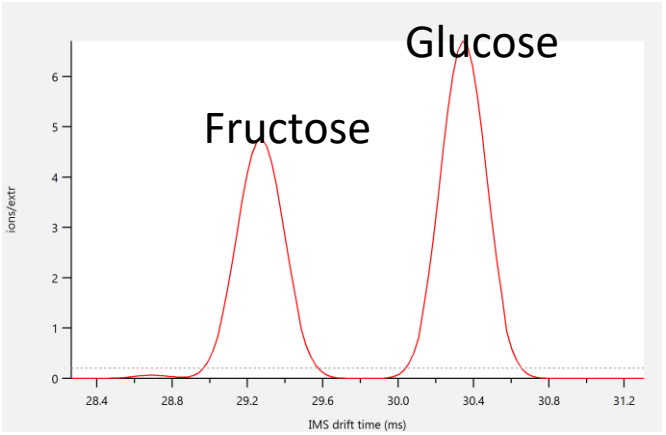
IMS can replace LC

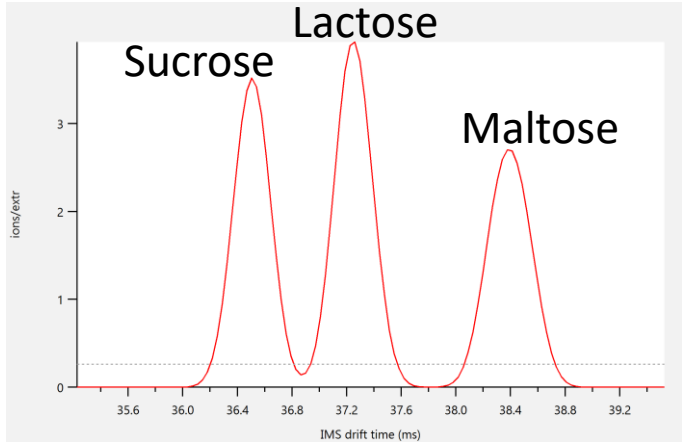


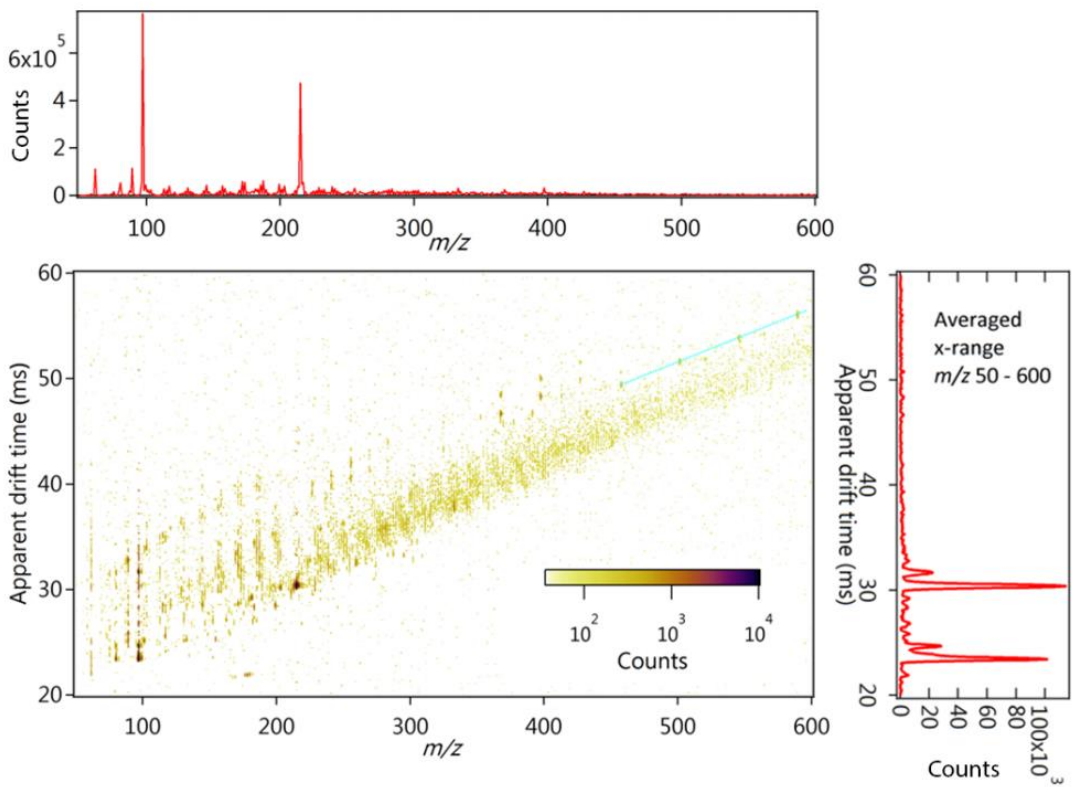
LC:
Run Time > 20 min



IMS:
1-min analysis!







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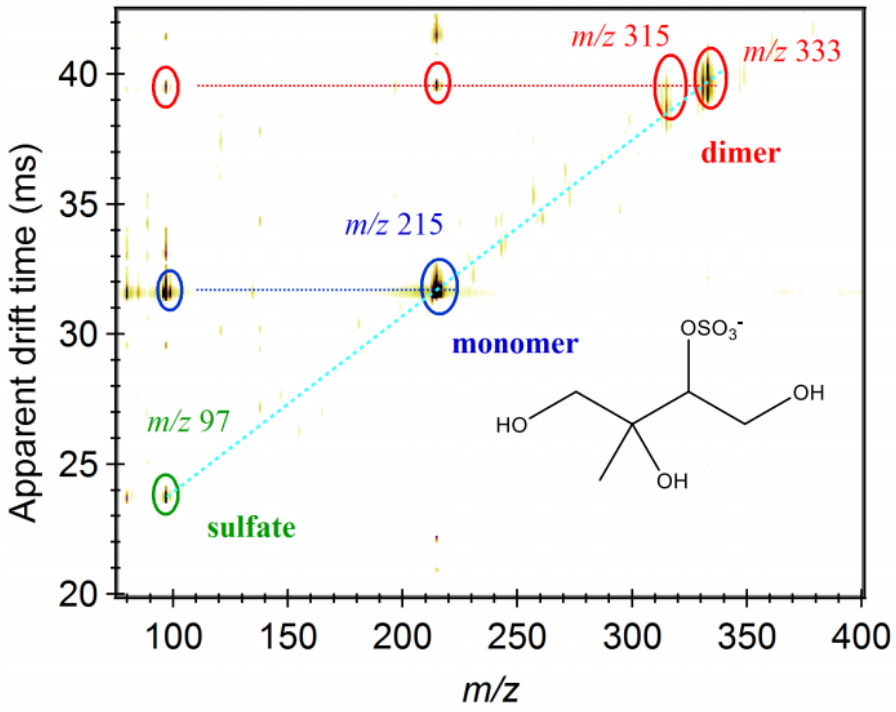
Atmospheric Measurement Techniques
Open Access
EGU

Ion mobility spectrometry–mass spectrometry (IMS–MS) for on- and offline analysis of atmospheric gas and aerosol species

Jordan E. Krechmer[1,2], Michael Groessl[3], Xuan Zhang[4], Heikki Junninen[5], Paola Massoli[4], Andrew T. Lambe[4,6], Joel R. Kimmel[3,4], Michael J. Cubison[3], Stephan Graf[3], Ying-Hsuan Lin[7,a], Sri H. Budisulistiorini[7,b], Haofei Zhang[7,c], Jason D. Surratt[7], Richard Knochenmuss[3], John T. Jayne[4], Douglas R. Worsnop[4,5], Jose-Luis Jimenez[1,2], and Manjula R. Canagaratna[4]

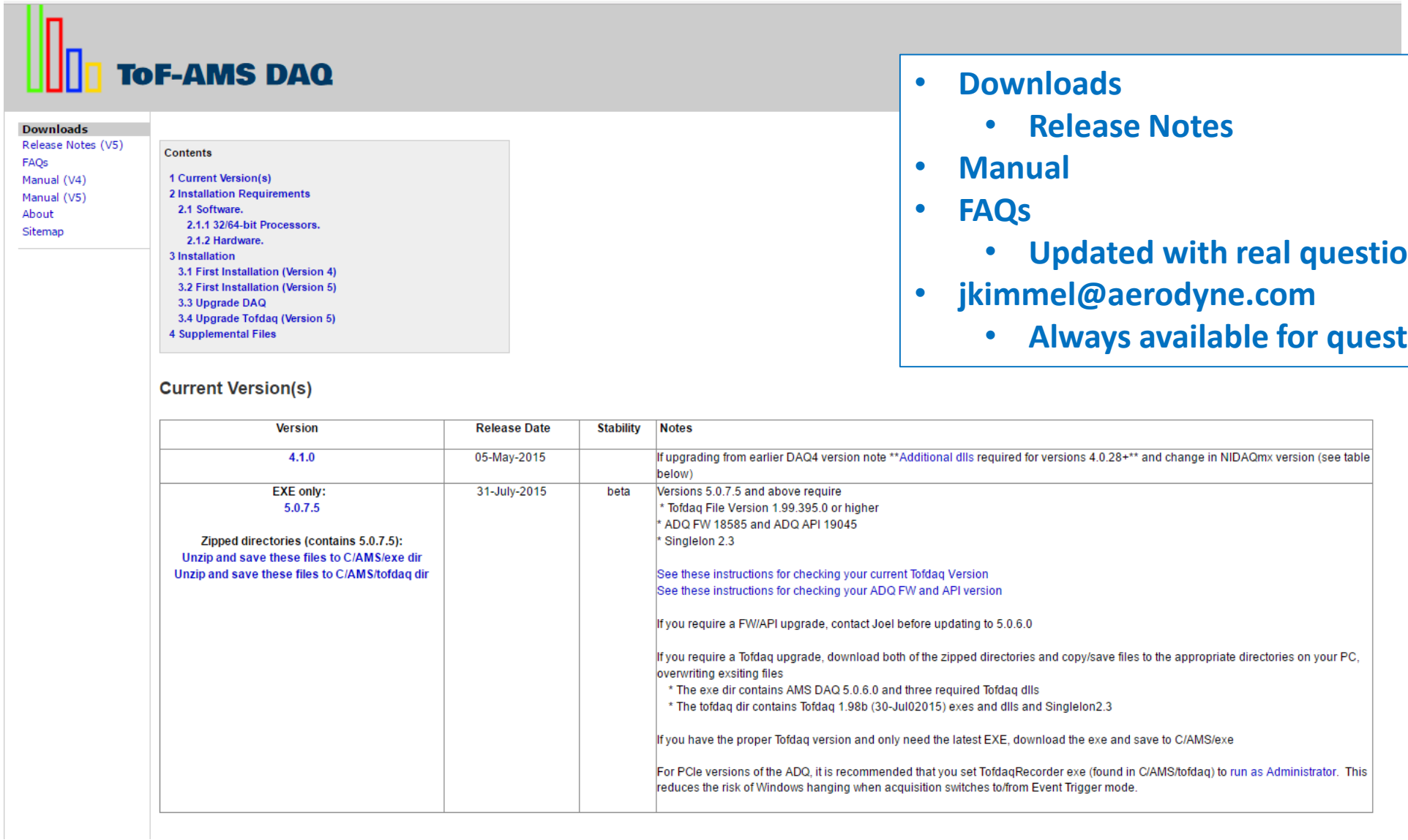


Application of IMS-MS in SOAS campaign

- Real-time gas-phase measurement with Nitrate CI
- Offline aerosol filter analysis using ESI. Resolution of WSOC isomers (not possible with MS alone)

Above: 2D IMS-MS of complex sample
Right: Oligomers align on 2D trend line; structure confirmed by CID

site.google.com/site/tofamsdaq



ToF-AMS DAQ

Downloads
Release Notes (V5)
FAQs
Manual (V4)
Manual (V5)
About
Sitemap

Contents

Current Version(s)

Version	Release Date	Stability	Notes
4.1.0	05-May-2015		If upgrading from earlier DAQ4 version note **Additional dlls required for versions 4.0.28+** and change in NIDAQmx version (see table below)
EXE only: 5.0.7.5 Zipped directories (contains 5.0.7.5): Unzip and save these files to C/AMS/exe dir Unzip and save these files to C/AMS/tofdaq dir	31-July-2015	beta	Versions 5.0.7.5 and above require * Tofdaq File Version 1.99.395.0 or higher * ADQ FW 18585 and ADQ API 19045 * Singlelon 2.3 See these instructions for checking your current Tofdaq Version See these instructions for checking your ADQ FW and API version If you require a FW/API upgrade, contact Joel before updating to 5.0.6.0 If you require a Tofdaq upgrade, download both of the zipped directories and copy/save files to the appropriate directories on your PC, overwriting exsiting files * The exe dir contains AMS DAQ 5.0.6.0 and three required Tofdaq dlls * The tofdaq dir contains Tofdaq 1.98b (30-Jul02015) exes and dlls and Singlelon2.3 If you have the proper Tofdaq version and only need the latest EXE, download the exe and save to C/AMS/exe For PCIe versions of the ADQ, it is recommended that you set TofdaqRecorder exe (found in C/AMS/tofdaq) to run as Administrator. This reduces the risk of Windows hanging when acquisition switches to/from Event Trigger mode.

- Downloads
  - Release Notes
- Manual
- FAQs
  - Updated with real questions!
- jkimmel@aerodyne.com
  - Always available for questions and suggestions

Latest Versions

Current Version(s)

Version	Release Date	Stability	Notes
4.1.0	05-May-2015		If upgrading from earlier DAQ4 version note **Additional dlls required for versions 4.0.28+** and change in NIDAQmx version (see table below)
EXE only: 5.0.7.5 Zipped directories (contains 5.0.7.5): Unzip and save these files to C/AMS/exe dir Unzip and save these files to C/AMS/tofdaq dir	31-July-2015	beta	Versions 5.0.7.5 and above require * Tofdaq File Version 1.99.395.0 or higher * ADQ FW 18585 and ADQ API 19045 * Singlelon 2.3 See these instructions for checking your current Tofdaq Version See these instructions for checking your ADQ FW and API version If you require a FW/API upgrade, contact Joel before updating to 5.0.6.0 If you require a Tofdaq upgrade, download both of the zipped directories and copy/save files to the appropriate directories on your PC, overwriting exsiting files * The exe dir contains AMS DAQ 5.0.6.0 and three required Tofdaq dlls * The tofdaq dir contains Tofdaq 1.98b (30-Jul02015) exes and dlls and Singlelon2.3 If you have the proper Tofdaq version and only need the latest EXE, download the exe and save to C/AMS/exe For PCIe versions of the ADQ, it is recommended that you set TofdaqRecorder exe (found in C/AMS/tofdaq) to run as Administrator. This reduces the risk of Windows hanging when acquisition switches to/from Event Trigger mode.

- **4.1.0:** Most widely used version on AP240 systems. No change in past 1 year.
- **5.0.7.5:** Latest release of DAQ5. (Sept 2016)
  - For DAQ5, also check Tofdaq versions, too

DAQ5 controls the new variety of hardware configurations

User interface adjusts based on combination of components in use

	DAQ4	DAQ5	
AP240	X	X	
NI6024E "Slow board"	X	X	DAQ5 also compatible with other NI cards
TPS1	X	X	
MS, PToF, FMS	X	X	
Light Scattering	X	X	*In beta for DAQ5 – runs simultaneous to ET*
ADQ1600		X	
ePToF		X	
mini-AMS		X	
TPS2		X	
Event Trigger SP Mode		X	
EyeON Electronics Box		X	
Time Resolved Chopper Movement (MS)		X	*In beta for DAQ5*
Auto-tuning		X	*Can be used without AMS DAQ; DAQ5 has some hand-shaking*

Control of New Electronic Box (EyeON)

- Replaces slow board
- Pump control to be added soon

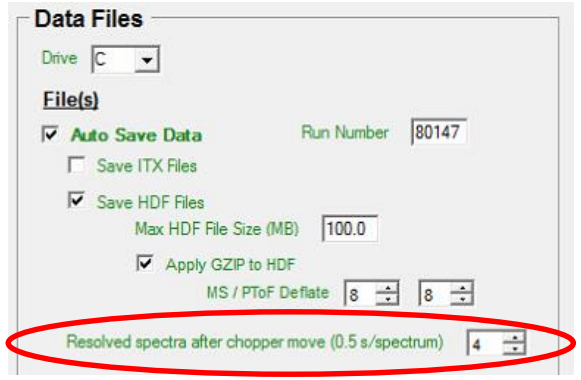
Time Resolved MS Data after Chopper Movement

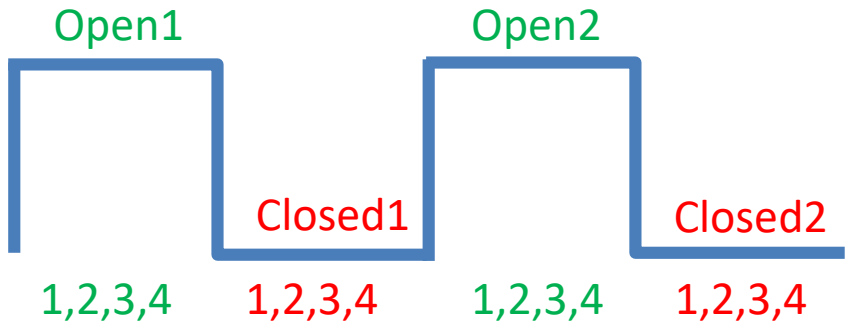
- New dataset added to HDF file structure. For each run, this dataset shows the first few seconds after chopper movement (for open and closed) with 0.5s resolution.

Light Scattering

- Light scattering data will be acquired simultaneous to Event Trigger SP. LS and MS data will be aligned in post processing based on timestamps of LS signals and recorded events.

Time-Resolved MS after Chopper Movement





Optionally enabled on Avg and Save Tab

In addition to saved MSopen and MSclosed data, creates _tr datasets, that resolve the first n spectra (0.5 s each) after the movement of the chopper

User defines number of resolved spectra, n, to save

Processing functionality included in Squirrel. All of this needs testing.

Standard Dataset:

MSopen = O1,1 + O1,2 + 01,3 + 01,4 + O2,1 + O2,2 + O2,3 + O2,4

Time Resolved Dataset:

MSopen_tr1 = O1,1 + O1,1

Msopen_tr2 = O1,2 + O1,2

Msopen_tr3 = O1,3 + O1,3

Msopen_tr4 = O1,4 + O1,4

Light Scattering

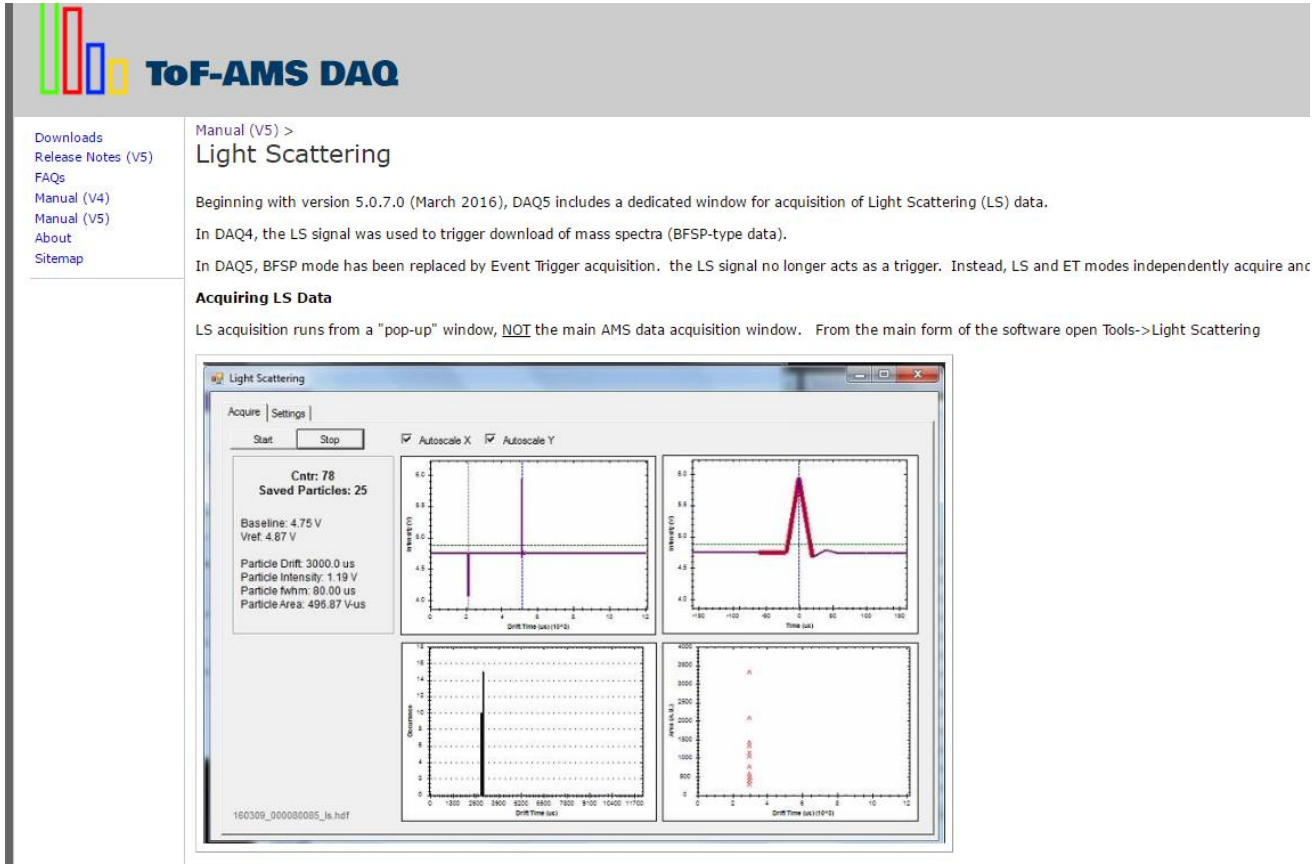
In DAQ4, LS was tightly coupled to BFSP mode. Used to trigger download of BFSP data.

In DAQ5, LS runs completely independent of AMS acquisition. Can run standalone or in parallel.

For single particle data, align LS pulses and Event Trigger events (particles) in post processing based on time stamps

This mode needs characterization and development!

See: https://sites.google.com/site/tofamsdaq/manual-v5/light-scattering



Event Trigger Single Particle Mode (ETSP)

Conceptually similar to BFSP

AMS data are filtered to save only those spectra that have user-defined features thought to represent particles.

Size determined by PToF time.

Reduced file size.

- 10 to 30x less data per particle than BFSP.

Extreme improvement in efficiency.

Single Particle Modes of AMS Depend on a Low Abundance Assumption

Specifically, 1 particle / chopper rotation

Above this limit we cannot assume recorded signals are single particles
"Saturation"

(This point can be reconsidered if we have LS)

Example of Saturation Limit:

For flow rate = 1.3 cc/s , 2% chopper duty cycle, 100 Hz

-> **50 particles/rotation** (For 2% -> 1 particle transmitted per rotation)
-> **5000 particles/sec** (100 rot/sec * 50 part/rot)
-> **3800 particles/cc** (5000 particles/sec * 1 sec/1.3 cc)

Particle Detection Efficiency

PDE = Particle Detection Efficiency

Best Case: Record every transmitted particle. PDE = Chopper Duty Cycle = 0.02

BFSP: PDE = 0.04 * 0.02 = **0.0008**

Bottlenecked by download of large data for every chopper

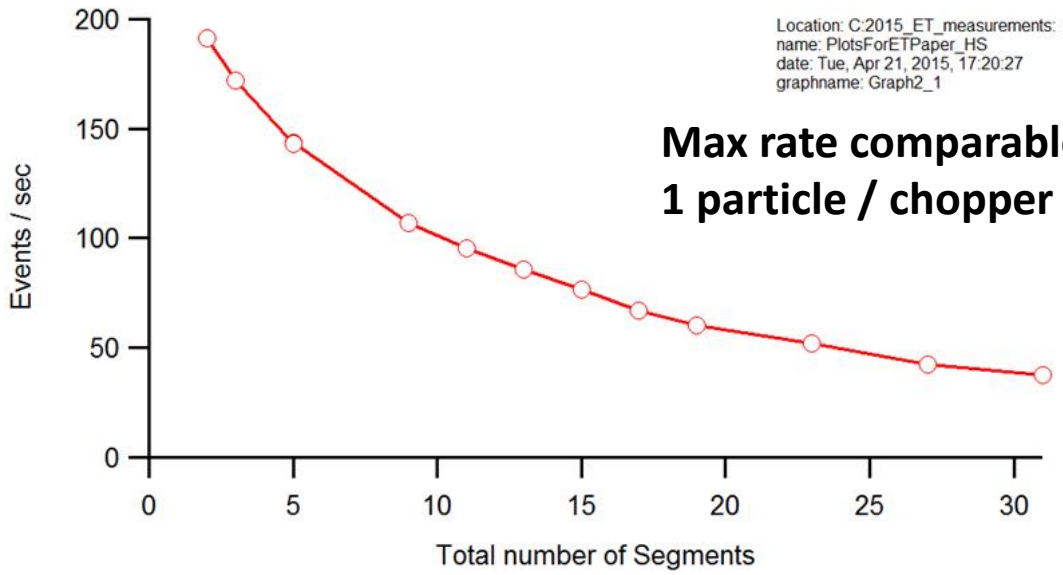
LS: 0.02 (very low concentration) to **0.0008** (High conc)

Only download chopper with particle

Download becomes bottleneck if lots of particles

Same as BFSP at high concentration

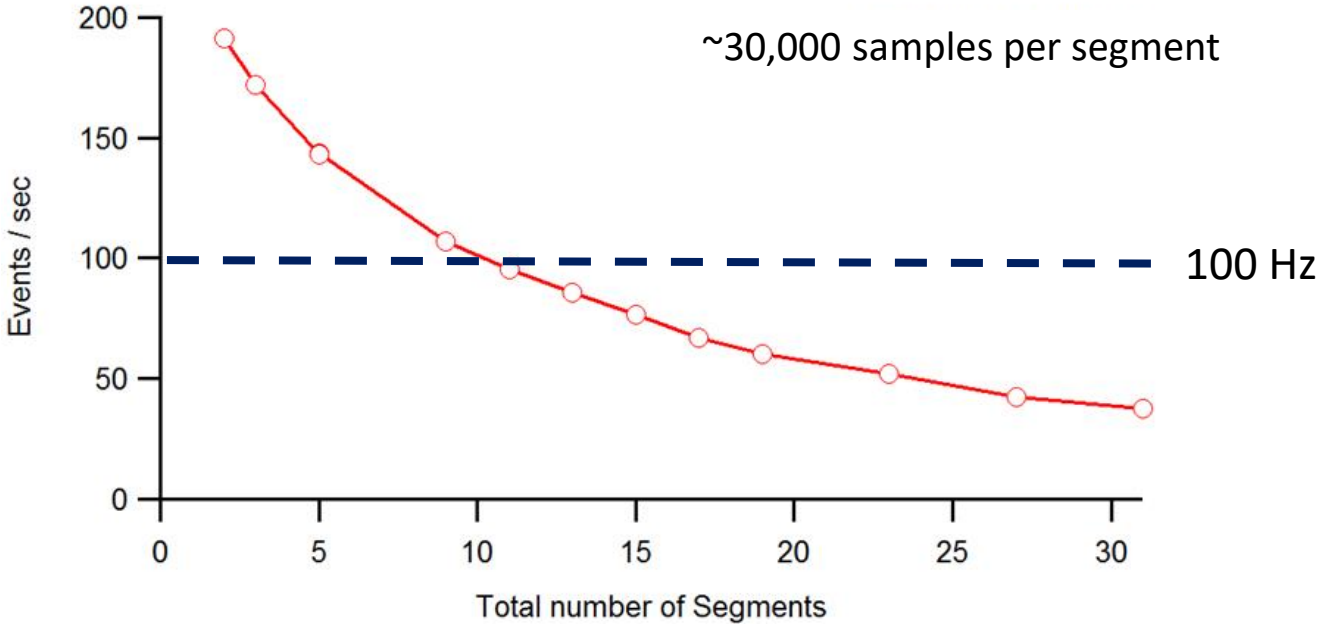
ET: 0.02

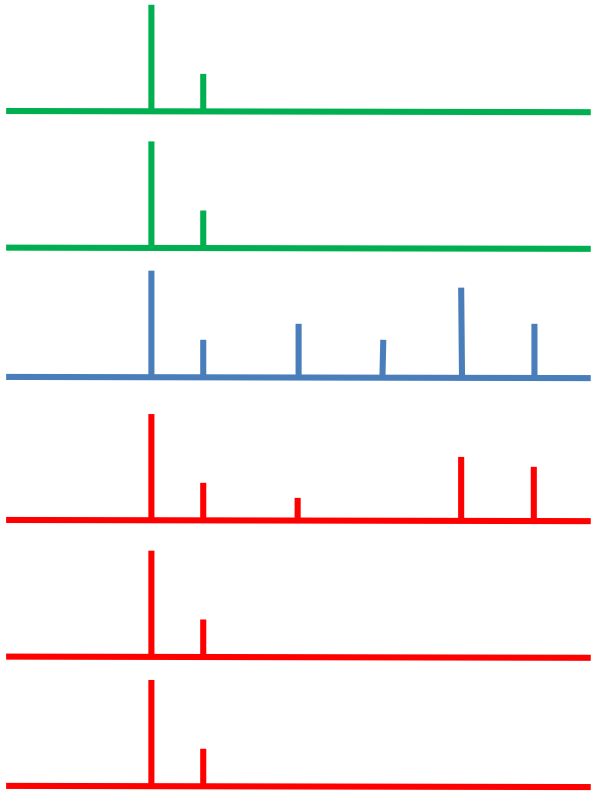


Max rate comparable to 1 particle / chopper

Maximum number of events/s as a function of number of segments/event. (Segment = spectrum). HTOF with ~30,000 samples per spectrum.

PDE for ET depends on data dimension





PDE in ET mode will depend on the size of the data per particle

Total data points per particle = (samples/segment) * Number segments

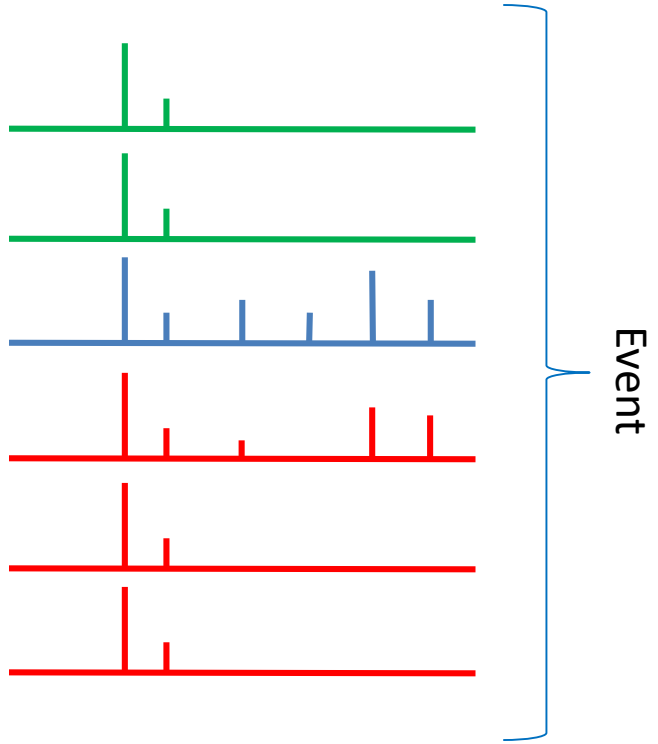
Number of samples determines mass range

Number of segments is also user adjustable (see right – we will come back to this)

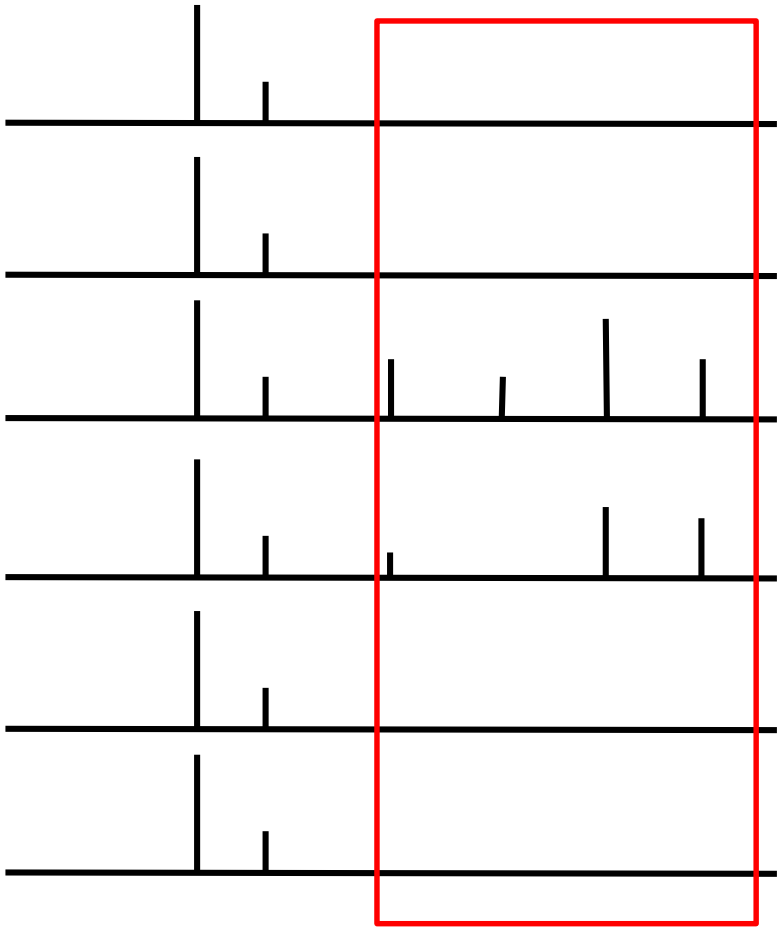
How we filter for particles

Event: A single MS extraction or series of consecutive extractions containing signals corresponding to the detection of a particle

- Single extractions are continuously acquired without averaging



How we filter for particles

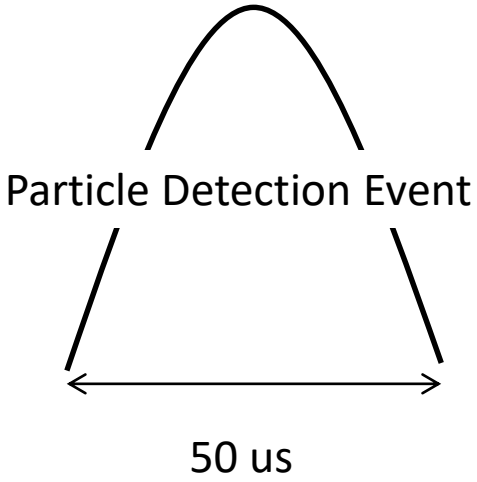


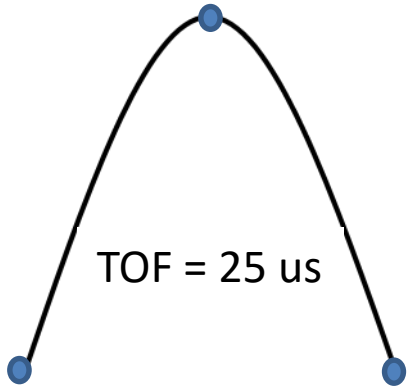
This idealized example

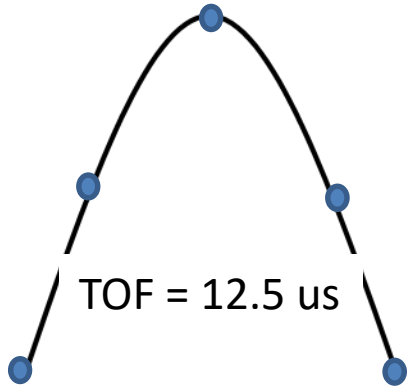
- Want to define an ROI that captures growing peaks in high mass range
- # of ions/event can be as low as 1 because there is no background

Real world considerations

- Location of large background peaks -> do we want these within ROI
- Summed background level in ROI -> affects # of ions / event
- Ionization efficiency: Small particles may produce very few ions and be harder to capture (see AN data from last year's UM)







We may be looking for a small number of ions at any given mass/charge

- Particularly small and/or mixed particles
- Ions/particle increases with pulse frequency. At expense of mass range

Capture as many particles as possible

The objective is to
CAPTURE as many particles as possible → Wide Net Filters

WITHOUT getting bogged down by false positives

We will use more sophisticated filtering in post-processing Don't need to sort particle types at the acquisition step and can also afford some false positives

**** This post-processing filtering could include LS data?!?**

Set trigger levels high enough to reject noise (or background) but low enough not to discriminate against small particles

Capture as many particles as possible

More considerations:

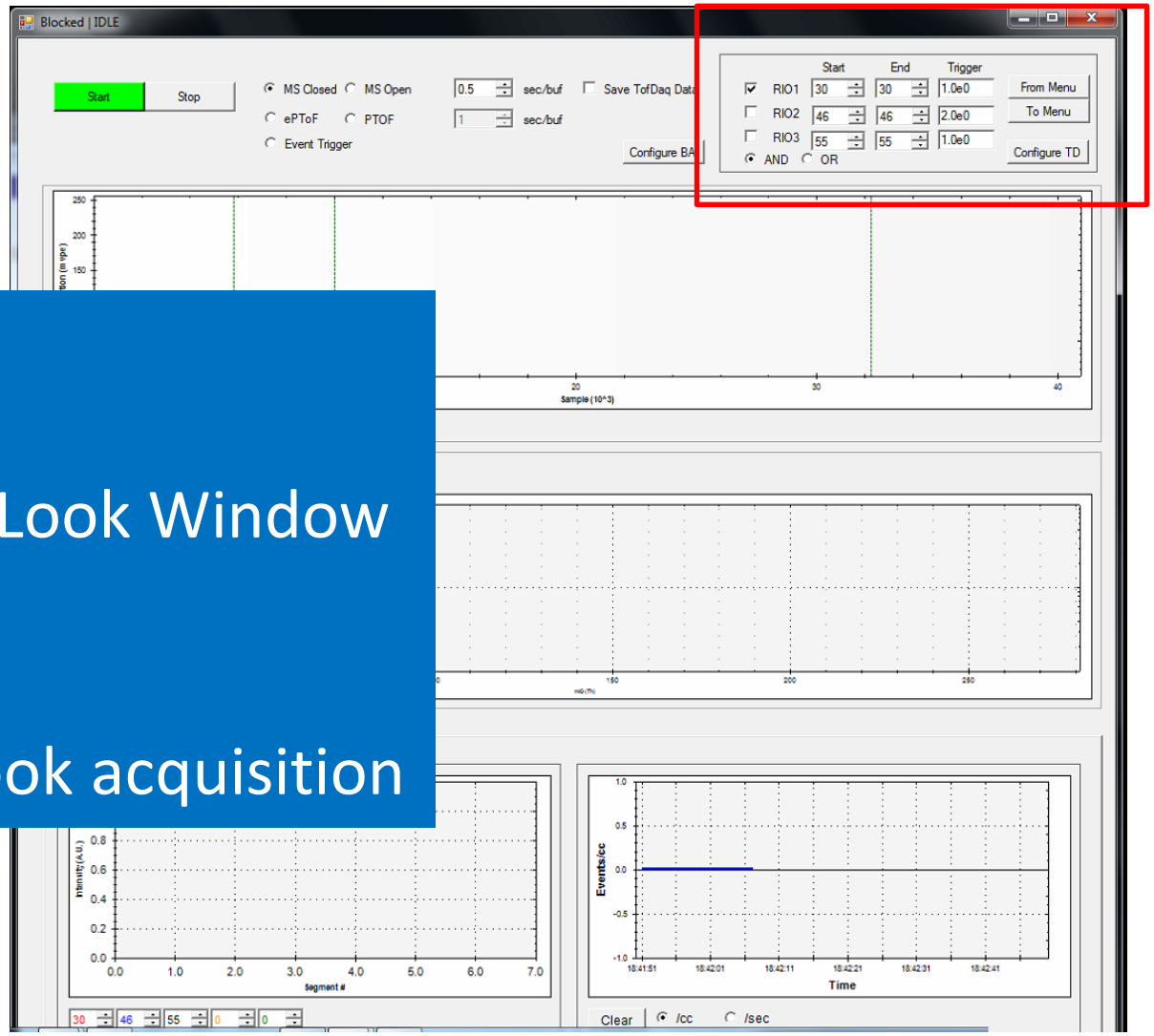
- User is pre-defining what a particle signal looks like
  - Must always acknowledge potential (pos and neg) bias
- Can we ever "know" that an event is a particle? Particularly small particle.
  - LS is a valuable confirmation
  - In post processing we can play with trigger levels, do statistical analysis of collection, compare size to # of ions recorded, etc …

Quick Look Window

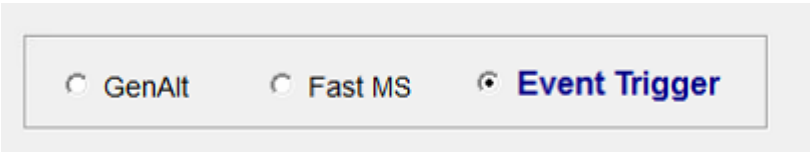
Experiment with ROI settings

Run ET-only experiments in the Quick Look Window (data are save!)

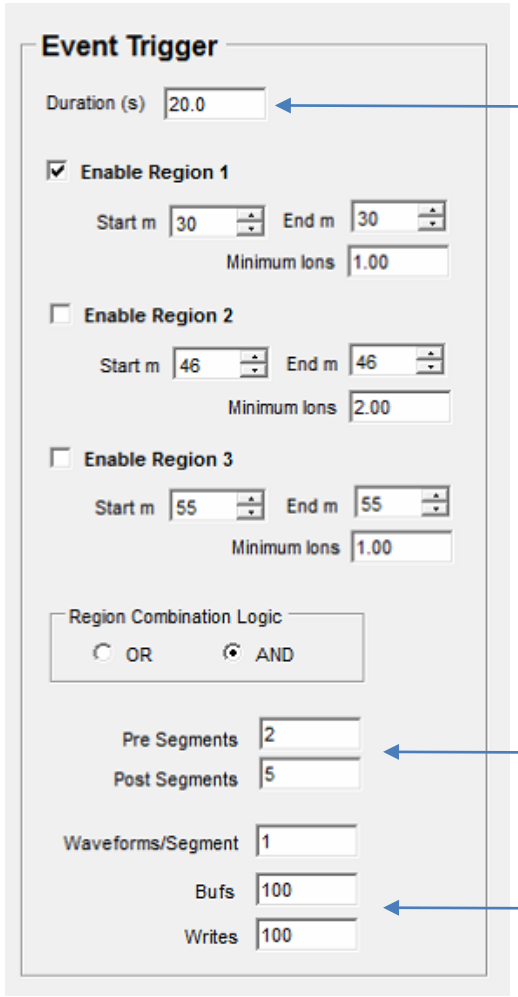
Run LS in parallel to GenAlt or QuickLook acquisition



Settings



A menu is defined as ET for Menu Switching



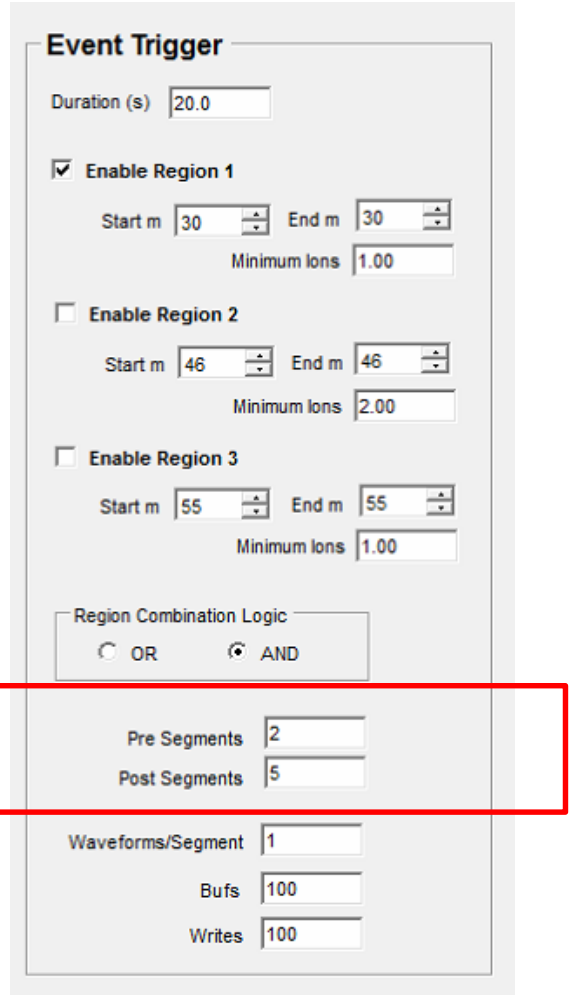
Amount of time to continuously acquire ET data

Define Event Filter

Define # of segments

Buf and Writes define length of an ET file
A file must have at least Event = Bufs in order to be readible

Segments



Recall that efficiency will go down as number of segments goes up

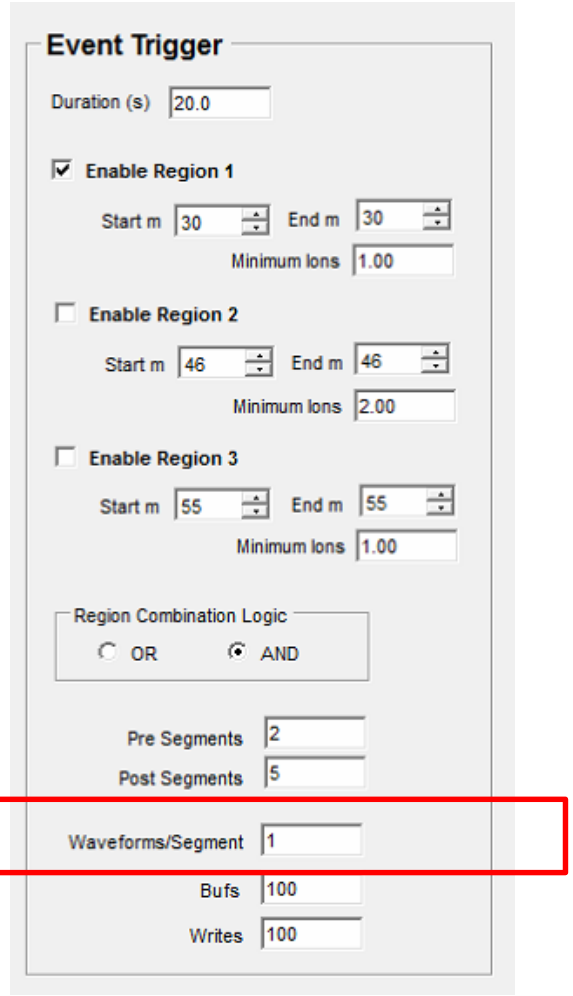
Firmware places some limits on number of segments

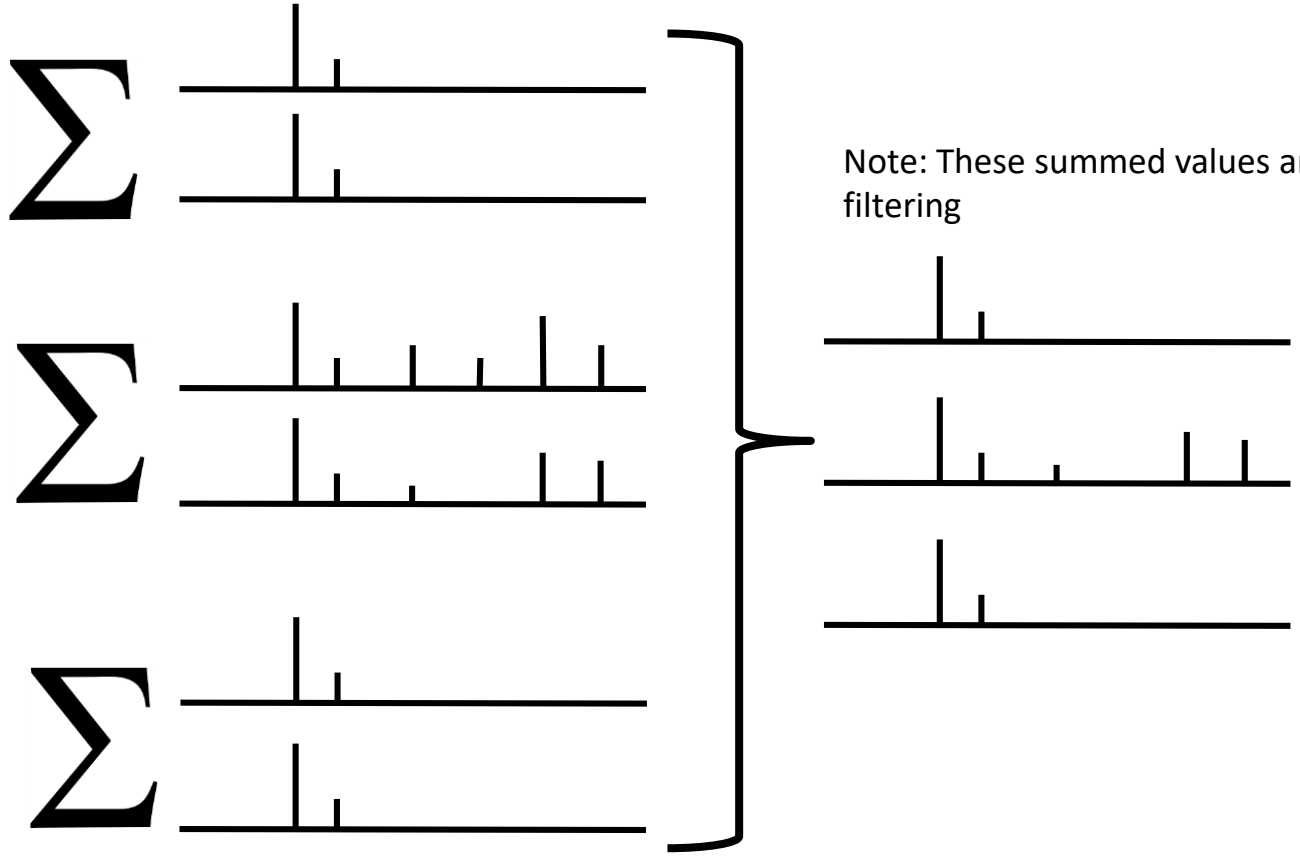
- **Total segments <= 255**
- **Pre segments <= 16**

Waveforms/Segments

waveform/segment value allows us to increase the duration of an event, while holding down number of segments

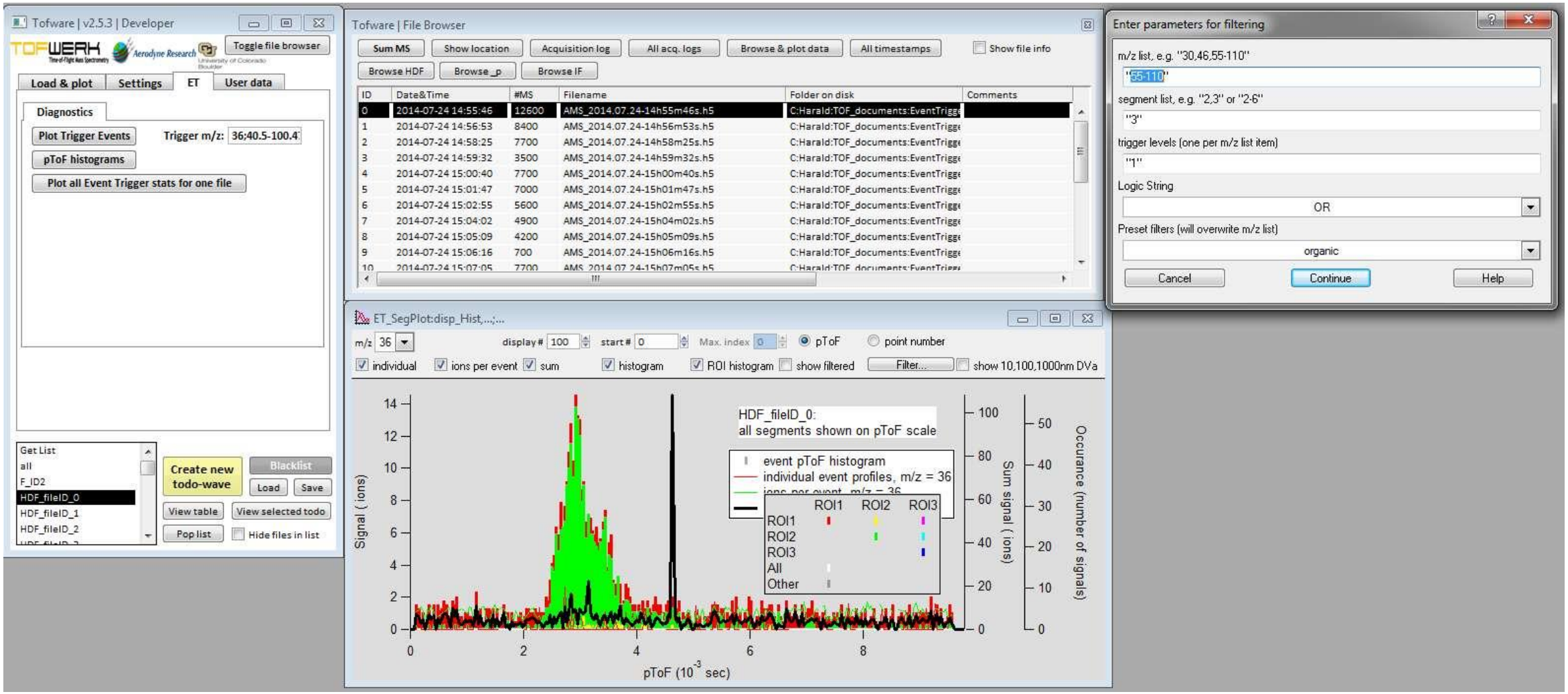
Same process as co-adding in PToF Mode

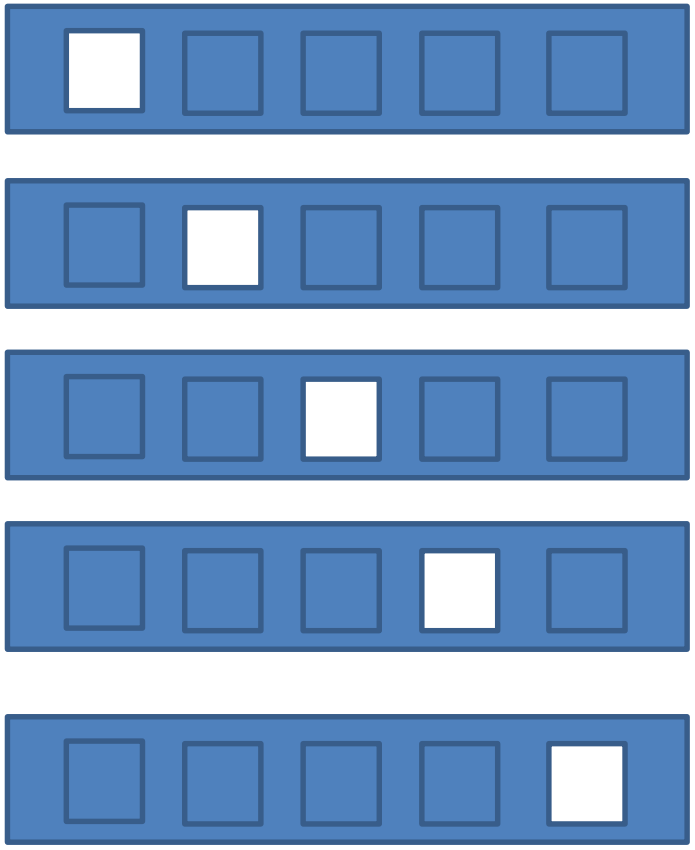




Note: These summed values are used for filtering

Dedicated Tool for ET Analysis





$I_1 = I_R$

$I_2 = I_G$

$I_3 = I_B$

$I_4 = I_Y$

$I_5 = I_P$

5 measurements to determine the intensity of 5 colors

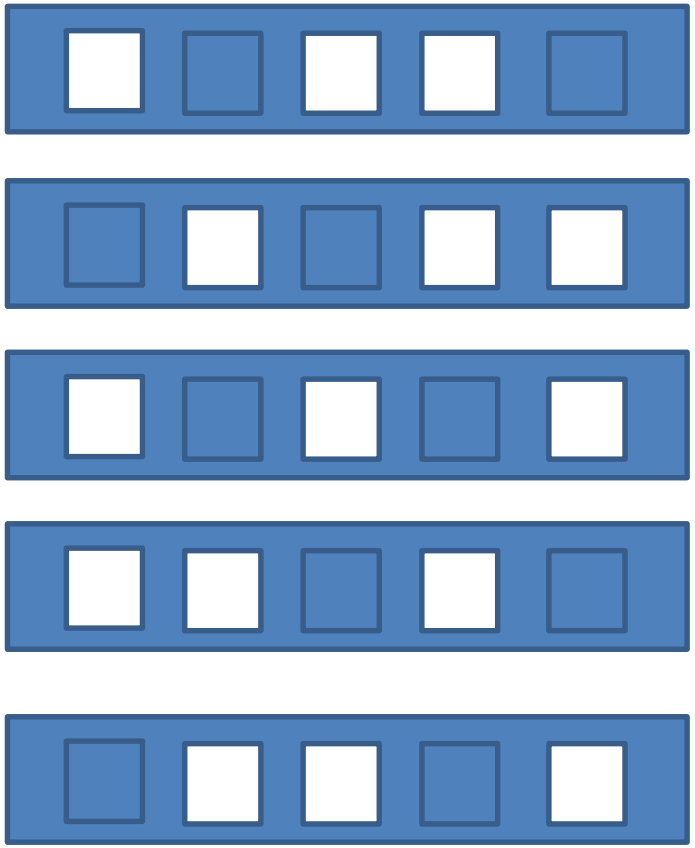
Single slit to ensure that at any given moment the detector sees only a single color

Straightforward interpretation of data: First measurement gives the intensity of red, etc

Total experiment duration = 5x the time required to make a single measurement

Each color measured during **20% or the total** experiment

*Note how sequence and signals shift linearly



$I_1 = I_R + I_B + I_Y$

$I_2 = I_G + I_Y + I_P$

$I_3 = I_R + I_B + I_P$

$I_4 = I_R + I_G + I_Y$

$I_5 = I_G + I_B + I_P$

5 measurements to determine the intensity of 5 colors

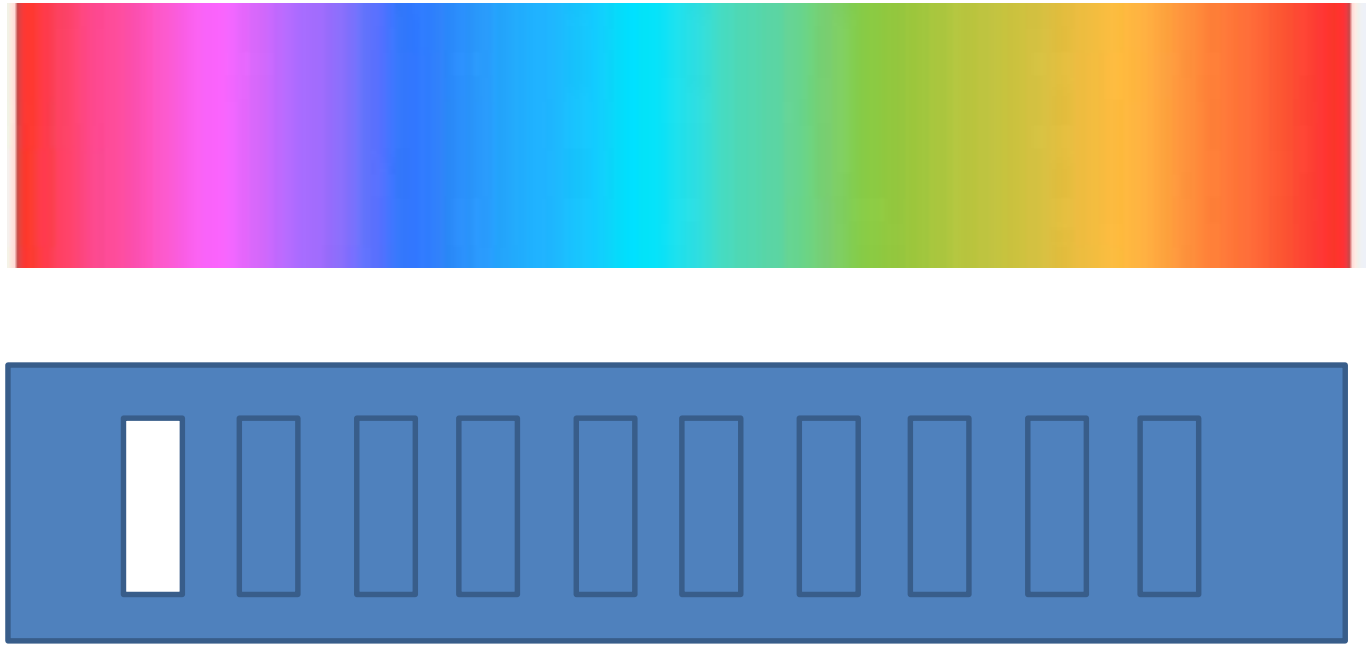
Multiple Slits Detector sees known combination of colors in each measurement.

Interpret signal by solving set of linear equations.

Total experiment duration same as single slit

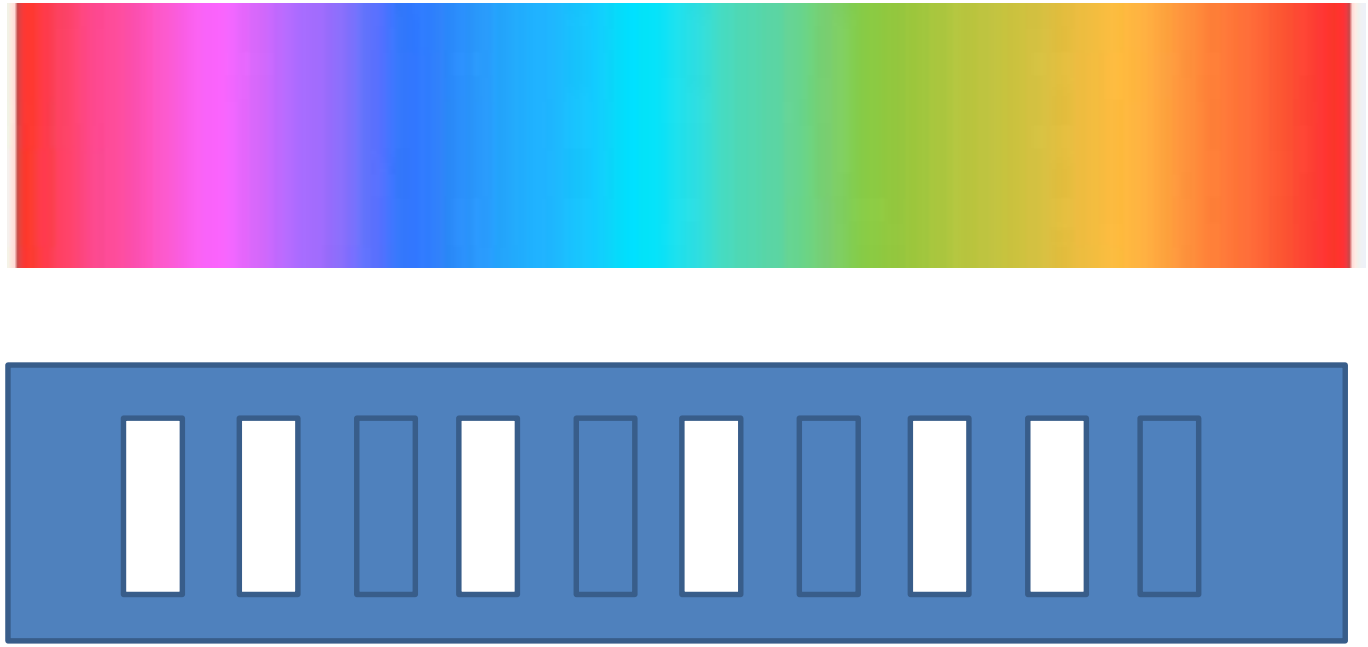
Each color measured with greater duty cycle than single slit ->

*Note how sequence and signals shift linearly



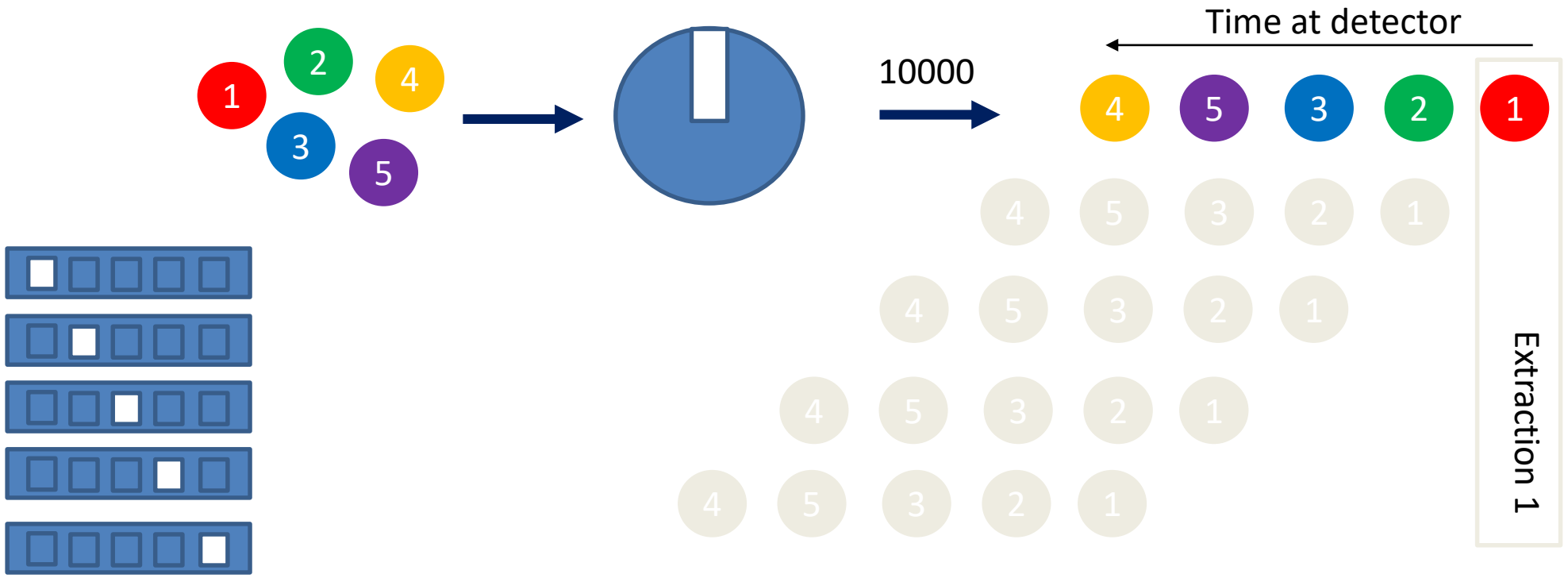
Single slit experiment has tradeoffs

- Increase resolution --> decrease time spent measuring any particular color



Multiplex decouples resolution and duty cycle

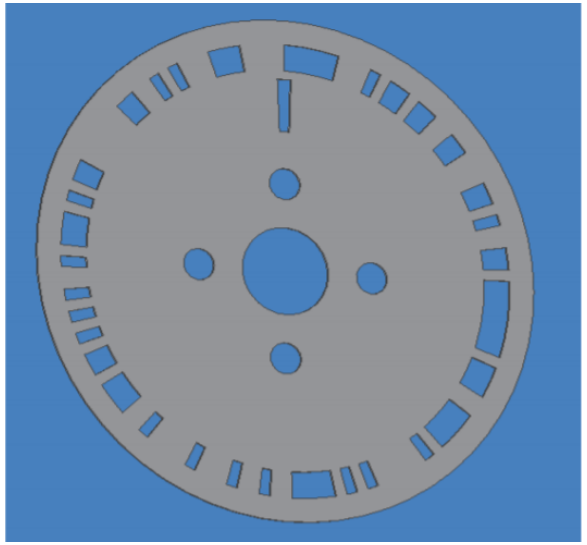
Decrease slit width, increase # of slits, maintain duty cycle

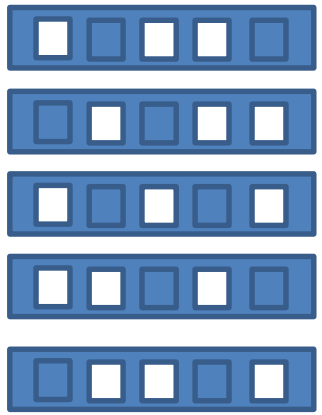


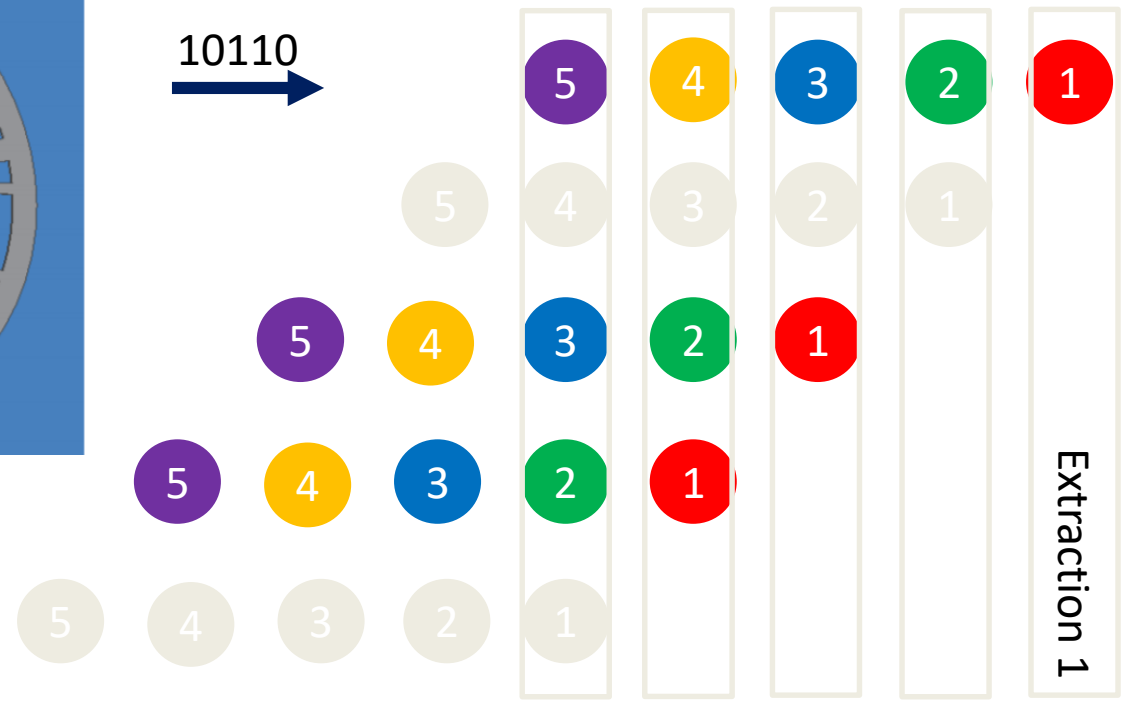
Like our spectroscopic mask, single slit modulates the signal so that only one particle size (color) strikes detector at any single time

Our detector is a single TOF measurement. In this example, we have 5 TOF/chop

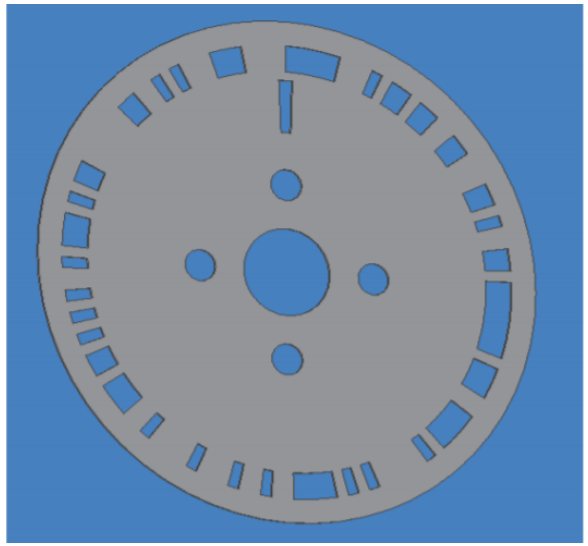
Extraction 1 measures PTOF1, and so on





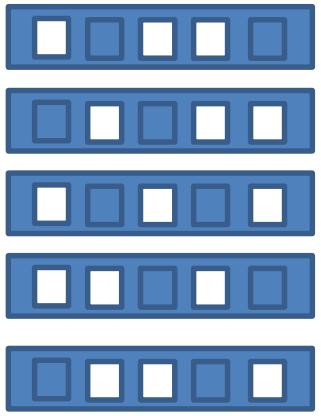


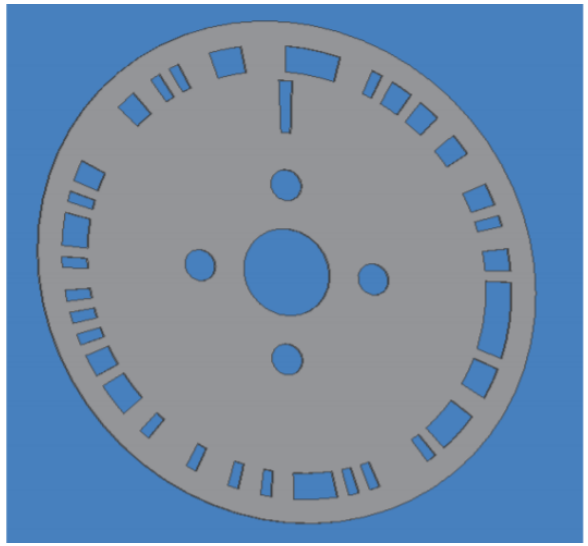
In the multiplexed ptof experiment, we introduce particles into the drift region with each slit opening. Multiple particle sizes from different slit opens can reach the TOF at the same time.



10110

In the multiplexed ptof experiment, the chopper rotates continuously, and the 5 TOF extractions are continuously averaged. -> wraparound of large particles to arrive in smaller extraction #s.





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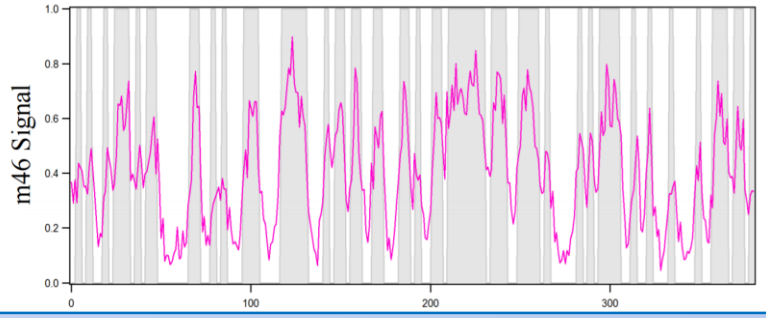
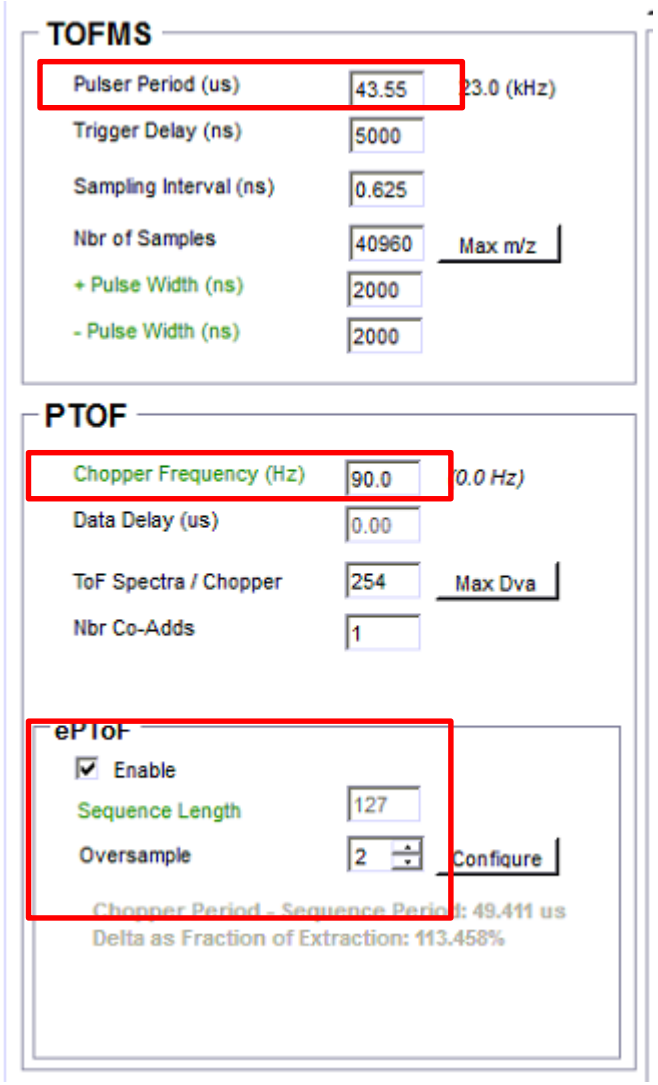


The averaged PTOF data must be deconvolved to recover the PTOF spectrum

ePToF Timing



ePTOF data are acquired in exactly the same manner as standard PTOF

Raw, encoded data waveform is saved. Deconvolved in Squirrel

Timing:

Requires exact synchronization between chopper and TOF

Our encoding sequence has 127 elements (open and closed slits)

We generally oversample by 2 → 254 TOF extractions per chopper rotation

For input chopper frequency, DAQ calculates pulser period

For more discussion of timing, see:
https://sites.google.com/site/tofamsdaq/manual-v5/menu-window/configuring-eptof