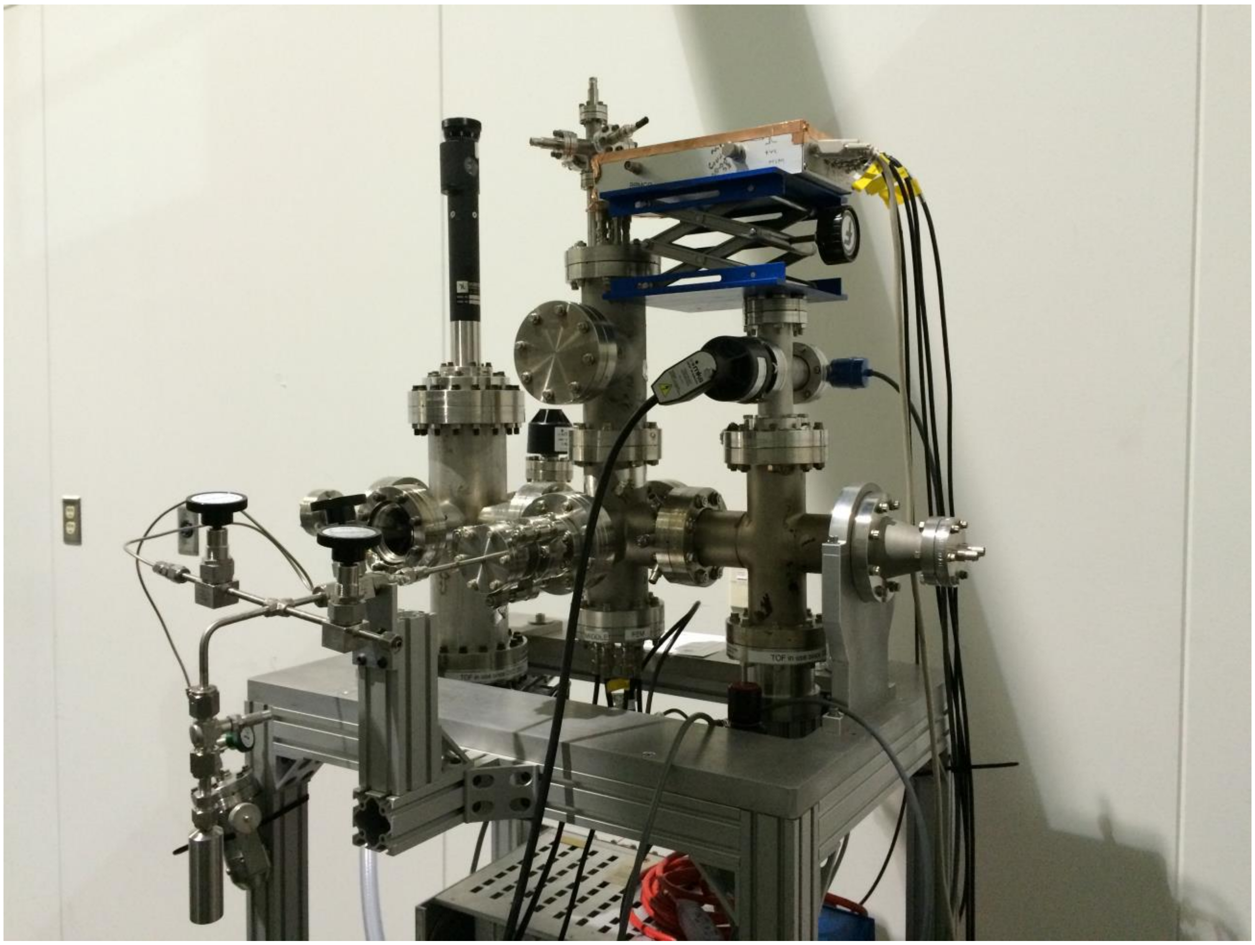
Time of Flight User Manual



Contents

Time-of-Flight User Manual

1. Structure of this manual

This manual starts with instructions on how to change the set voltages and how to collect data (with comments on the file structures produced), followed by a typical mass spectrum. This is what users will spend most of their time referring to. These sections are followed by sections on connecting the high voltages, the signal processing and signal connections and behind the scenes settings. These are intended for troubleshooting and for beamline staff. This manual should be read alongside the beamline Users Manual.

(http://exshare.lightsource.ca/vlspgm/Pages/Manuals.aspx)

2. Introduction

The Time of Flight Mass Spectrometer (TOF) available at the Canadian Light Source(CLS) follows the Wiley-McLaren design [1]. Dimensions and precise details can be found in Guerra *et. al.* [2] Figure 1 shows a sketch of the instrument, with relevant dimensions being given in Table 1. The TOF is an “electron start - ion stop” system equipped with multi-hit electronics and thus uses constant voltages (not pulsed). It is capable of recording photoionization induced mass spectra and PEPIPICo maps (Photo-Electron Photo-Ion Coincidence maps) with no bias in the photoelectron start or ions collected for photoelectrons up to 200eV kinetic energy.

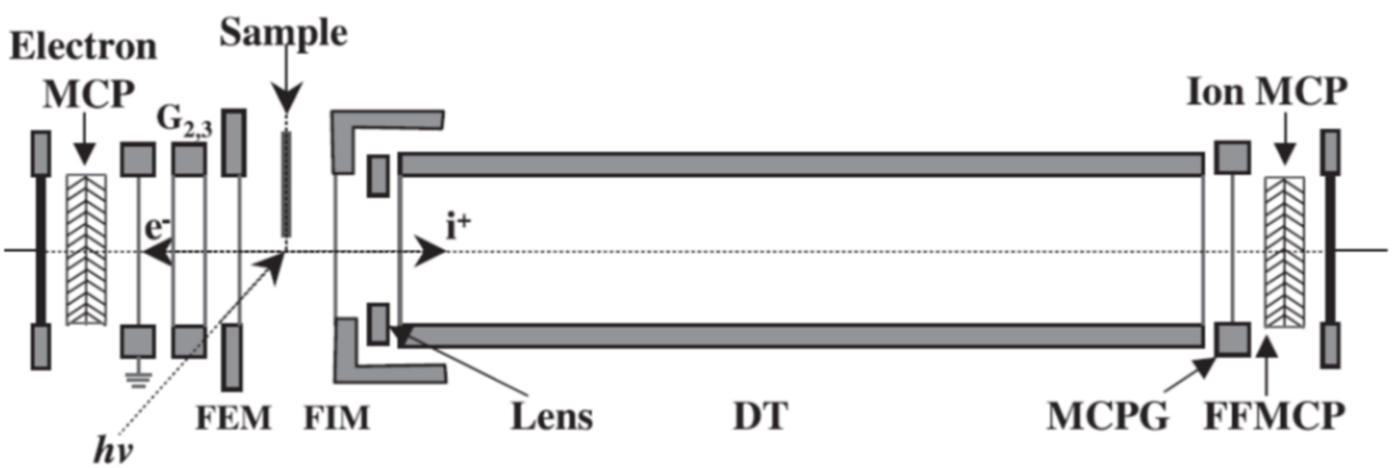


Figure 1. Schematic diagram of the experimental TOF apparatus.

Geometrical Feature	Dimension / mm
FEM – FIM gap	20
FIM – Lens Gap	5
Lens – Front DDT	10
DT Length	232

Table 1 Dimensions for the experimental TOF apparatus.

The anode behind the ion drift tube and MCP is split in half and the signal from each half may be processed separately. They are referred to as Ion 1 and Ion 2 in this manual.

The apparatus also contains a filter rack, to remove any second order contribution from the incoming light over certain energy ranges. The filter rack contains a 150nm Aluminium (Al) filter and 160nm Tin (Sn) filter. It also contains a slit which can be used to reduce the scattered light in the apparatus. The position of the filter rack is controlled by the linear motion drive above the differential section of the Time of Flight Apparatus.

Filter / Slit	Setting Position
Sn Filter	32.0 mm
Al Filter	17.5 mm
Slit (2mm x 12.5mm)	4 mm

Table 2 Settings of filters in the filter rack

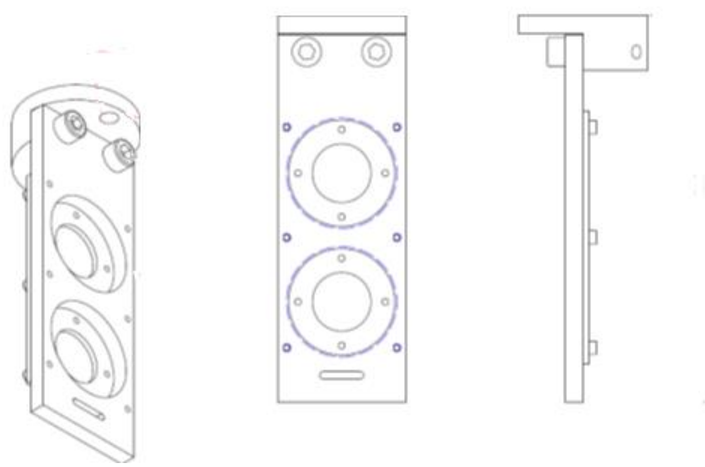


Figure 2 the filter rack as part of the Time of Flight apparatus.

3. *Setting the voltages.*

Assuming that the apparatus is properly set up and that the beamline is open and with the correct photon energy, then the first step in collecting data is to double click on the "Time of Flight" icon. This opens a folder containing various programs (shown below). At this point double clicking on the "Time of Flight desktop" icon starts the program (highlighted in the screengrab with a black box). Further details on setting up the apparatus and using the beamline can be found later in this manual and in the beamline Users Manual.

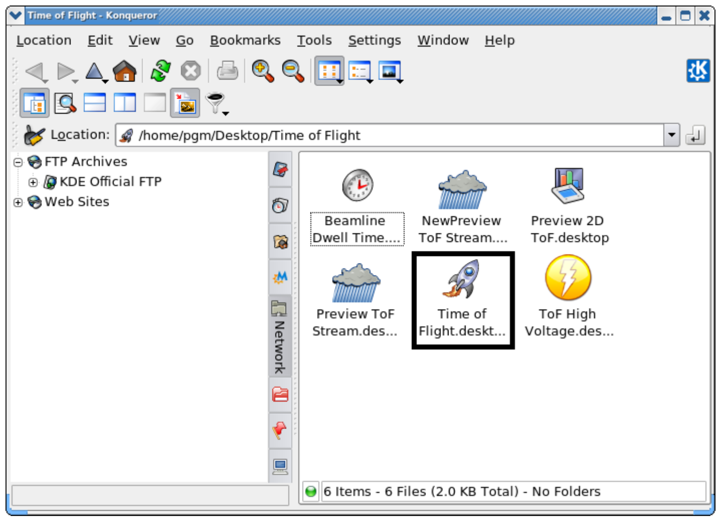


Figure 3. The "Time of Flight" icon (left) and the folder it opens (right)

When the program starts the "Time of Flight Controls GUI" appears.

Clicking on the "HV" button in the "Time of Flight Controls" GUI (Yellow button at the top left on the right hand GUI in figure 5 below) will bring up the "PGM ToF HV GUI". This sets all the voltages required for running the time of flight. They are split into two groups "Ions", setting the negative voltages and "Electrons", setting the positive voltages. <u>The value to be entered and the value returned is the absolute value of the voltage</u>. Each group has the ability to control the ramp up and ramp down rate of the group of voltages.

Figure 4. The “Time of Flight Controls” GUI (left) and the “PGM ToF HVs” GUI (left).

Ions

Do not turn on the voltages until the pressure in the Time of Flight apparatus is better than 5×10^{-6} Torr.

Ramp up rate: This should be set to 2V/s for the first time the High voltages are applied since the apparatus has been pumped down. Otherwise this is normally left at 20 V/s.
Ramp down rate: This should be set to either 20 V/s or 50 V/s.

Ion Voltages: This is where the voltages on the “ion side” of the apparatus are set. Each voltage can be set to be part of the ion group and thus ramped up at the constant rate of the group with a common start point. Clicking on the “In Group” box turns group membership on or off (green Y check box or red N check box). The requested voltage is set in the “Setpoint” box, and the actual voltage is indicated under the actual voltage column. The current drawn in supplying the voltage is indicated in the “Measured Current Column”. (The “Current” box at the top right of the controls indicates the value of the largest of the individual currents.) The “delta” control box allows the setting of a step by which the voltage will be increased or decreased each time the neighbouring “up” or “down” button is clicked.

Ion Currents: The MCP Front should read a current of approximately 130 µA for a voltage of approximately 4kV. The MCP Back should read a current of approximately 45 µA for a voltage of approximately 1.65kV.

On: Once the desired voltages are set they may be activated by pressing the “On” button. The voltages that are checked as part of the group will then ramp up together art the requested ramp up rate. The description will change from “Off” to “Ramping Up” and then to “On”.

Off: Clicking the “Off” button will ramp down all the voltages in the group at the chosen ramp-down rate. The description will change from “On” to “Ramping Down” to “Off”.

Changing Voltages: One may change the voltages when they are on. To do this either click the appropriate “up” or “down” button or type a new voltage into the “Setpoint” box and press enter. The voltage will then ramp up or down at the relevant ramp rate until it reaches the requested value.

Ion Ground: This should be set at 0.0 and removed from the group. The physical (SHV) connection should be connected with a shorting cable to the system ground.

MCP Voltages: The maximum voltage applied to the ion MCP is 2.4kv. The voltage applied to the ion MCP is Ion MCP back minus Ion MCP Front.

<u>Electrons</u>

Do not turn on the voltages until the pressure in the Time of Flight apparatus is better than 5×10^{-6} Torr.

Ramp up rate: This should be set to 2V/s for the first time the High voltages are applied since the apparatus has been pumped down. Otherwise this is normally left at 20 V/s.
Ramp down rate: This should be set to either 20 V/s or 50 V/s.

Electron Voltages: This is where the voltages on the “electron side” of the apparatus are set. Each voltage can be set to be part of the electron group and thus ramped up at the constant rate of the group with a common start point. Clicking on the “In Group” box turns group membership on or off (green Y check box or red N check box). The requested voltage is given in the “Setpoint” box, and the actual voltage is returned under the actual voltage column. The current drawn in supplying the voltage is returned in the “Measured Current Column”. (The “Current” box at the top right of the controls returns the value of the largest of the individual currents.) The “delta” control box allows the setting of a step by which the voltage will be increased or decreased each time the neighbouring “up” or “down” button is clicked.

Electron Currents: e- MCP should read a current of approximately 70 µA for a voltage of approximately 2.4kV.

On: Once the desired voltages are set they may be activated by pressing the “On” button. The voltages that are checked as part of the group will then ramp up together art the requested ramp up rate. The description will change from “Off” to “Ramping Up” and then to “On”.

Off: Clicking the “Off” button will ramp down all the voltages in the group at the chosen ramp-down rate. The description will change from “On” to “Ramping Down” to “Off”.

Changing Voltages: One may change the voltages when they are on. To do this either click the appropriate “up” or “down” button or type a new voltage into the “Setpoint” box and press enter. The voltage will then ramp up or down at the relevant ramp rate until it reaches the requested value.

e- Floating Bias: This should be set at 0.0 and removed from the group. The physical (SHV) connection should be connected with a shorting cable to the system ground.

MCP Voltages: The maximum voltage applied to the electron MCP is 2.4kV

4. *Collecting Data*

Clicking the “Graph” button on the “Time of Flight Controls” screen (figure 4) will bring up the “Multihit TDC GUI” screen (figure 5). From here one can take single TOF mass spectra or one can collect multicoincidence spectra (e.g. PEPIPICo), through the ASCII stream option. Data will be recorded at the current photon energy controlled by the beamline program.

4.1 Collecting a single Time of Flight Mass Spectrum

The gas pressure and photon flux should be adjusted so that the ion and electron count rates are below approximately 30 kHz. The photon energy and exit slit widths are controlled by the “PGM Control Panel” GUI as described in the Users Manual. The count rates can be read either from the ratemeters in the NIM bin below the apparatus or by opening the “PGM Scaler” GUI by double clicking on the “PGM Scaler” icon on the home desktop (figure 5). Channel 0 gives the electron counts, channel 1 gives the Ion 1 counts and channel 3 gives the Ion 2 counts in a specified time interval.

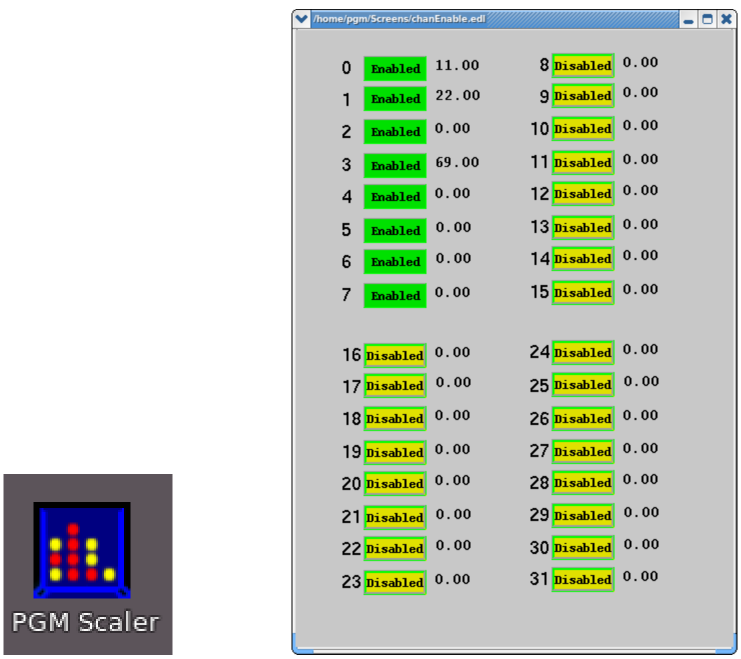


Figure 5 the “PGM Scaler” icon and “PGM scaler GUI.

The specified time interval over which the scaler counts are integrated can be set by opening the “Synchronized Dwelltime Controls" GUI by double clicking on the “Beamline Dwell Time” icon on the home desktop (figure 6). The integration time is set in the “Dwell Time” box in the top line of the “Synchronized Dwelltime Controls” GUI.

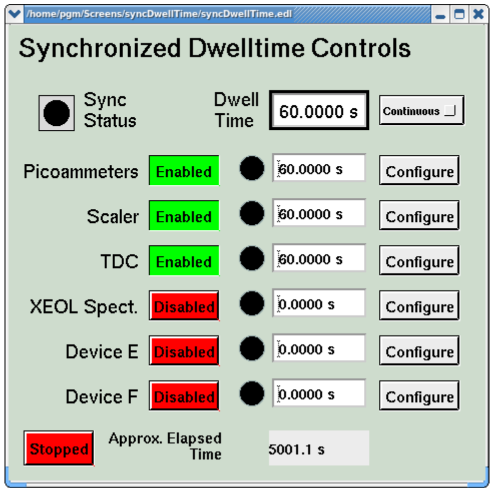


Figure 6 the “Beamline Dwell Time” icon and “Synchronized Dwelltime Controls” GUI.

4.2 Collecting a single Time of Flight Mass Spectrum

Clicking the “Graph” button on the “Time of Flight Controls” GUI (figure 4) will bring up the “Multihit TDC” GUI screen (figure 7). To collect a single mass spectrum perform the following procedure.

- Set the desired Integration Time. (“Integration Time” box in “Multihit TDC” GUI – figure 7).
- Set event data to “No Stream”. (Yellow button bellow “Event data as” in “Time of Flight Controls” GUI – figure 4 – which can take the values “No Stream”, “ASCII Stream” or “Binary Stream”.)
- Set “TDC Engine” to “Running”. (Either by clicking the button below “Engine” in the “Time of Flight Controls” GUI or by clicking the below “TDC Engine Mode” in the “Multihit TDC” GUI. This can take the values “Running” or “Stopped”).
- Set “Integrate” to “Running” – this will start the data collection. (Click the button below “Integrate” in the “Multihit TDC” GUI – figure 7. This can take the values “Running” or “Stopped”.

While the data is collecting, one can click “Update” on the “Multihit TDC” GUI to display the latest data. Further controls on this GUI are:

Rebin: One can choose to rebin the data to reduce apparent noise.
Linear/Log: One can chose to display the ordinate data in a linear or log scale.
Spectrum: One can choose to plot either Ion 1 data (1) or Ion 2 data (2).
Display ROIs: One can set various **R**egions **Of** **I**nterest. This is useful when recording partial ion yield spectra. A maximum of 8 are saved in the partial ion yield spectra.

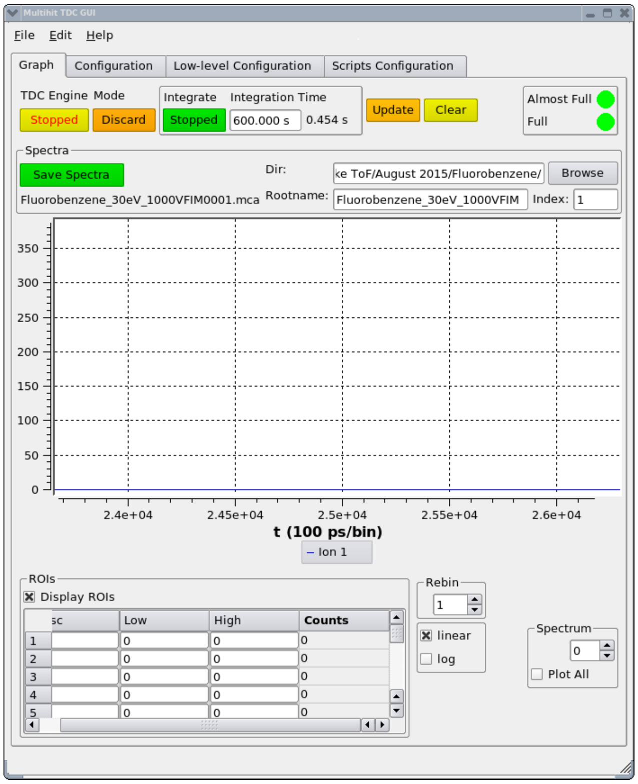


Figure 7. The “Multihit TDC” GUI

After the data is collected one can save the data. Referring to the “Multihit TDC” GUI (figure 7)

- Click “Browse” to set the directory in which the data will be saved.
- Type the root name of the file in the “Rootname:” box and set the index number. The index number will increment each time a file is saved.
- The file will be saved as Rootname0001.mca etc.

4.2.1 File structure of single .mca files

The file structure of the .mca files is

```
# TDC spectra
# Thu Aug 20 09:26:17 2015
# TDC Resolution = 100 ps
# Coincidence Window Width = 5.000 us (200 units)
# Coincidence Window Offset = -4.875 us (-195 units)
# x   ch0   ch4   ch8   ch12
0.000000 30 27 0 2730820
1.000000 35 8 0 0
2.000000 58 2 0 0
3.000000 58 0 0 0
4.000000 61 0 0 0
…
99996.000000 0 0 0 0
99997.000000 0 0 0 0
99998.000000 0 0 0 0
99999.000000 0 0 0 0
```

Column 1 is the Time of flight in units given in line 3 "TDC Resolution"
Columns 2 and 3 are the counts collected on each half of the split anode collector.
The last entry in the column at time 0.00000 is the total number of events.

4.3 Recording single Multicoincidence Spectra

Single Multicoincidence (PEPIPICo) images can be recorded. (**P**hoto**E**lectron **P**hoto**I**on Photo**I**on **Co**incidence.) This is accessed via the “New Preview TOF Stream Desktop” icon in the “TOF Folder” (Figure 3). This brings up the “ToF Stream Analyzer” GUI.

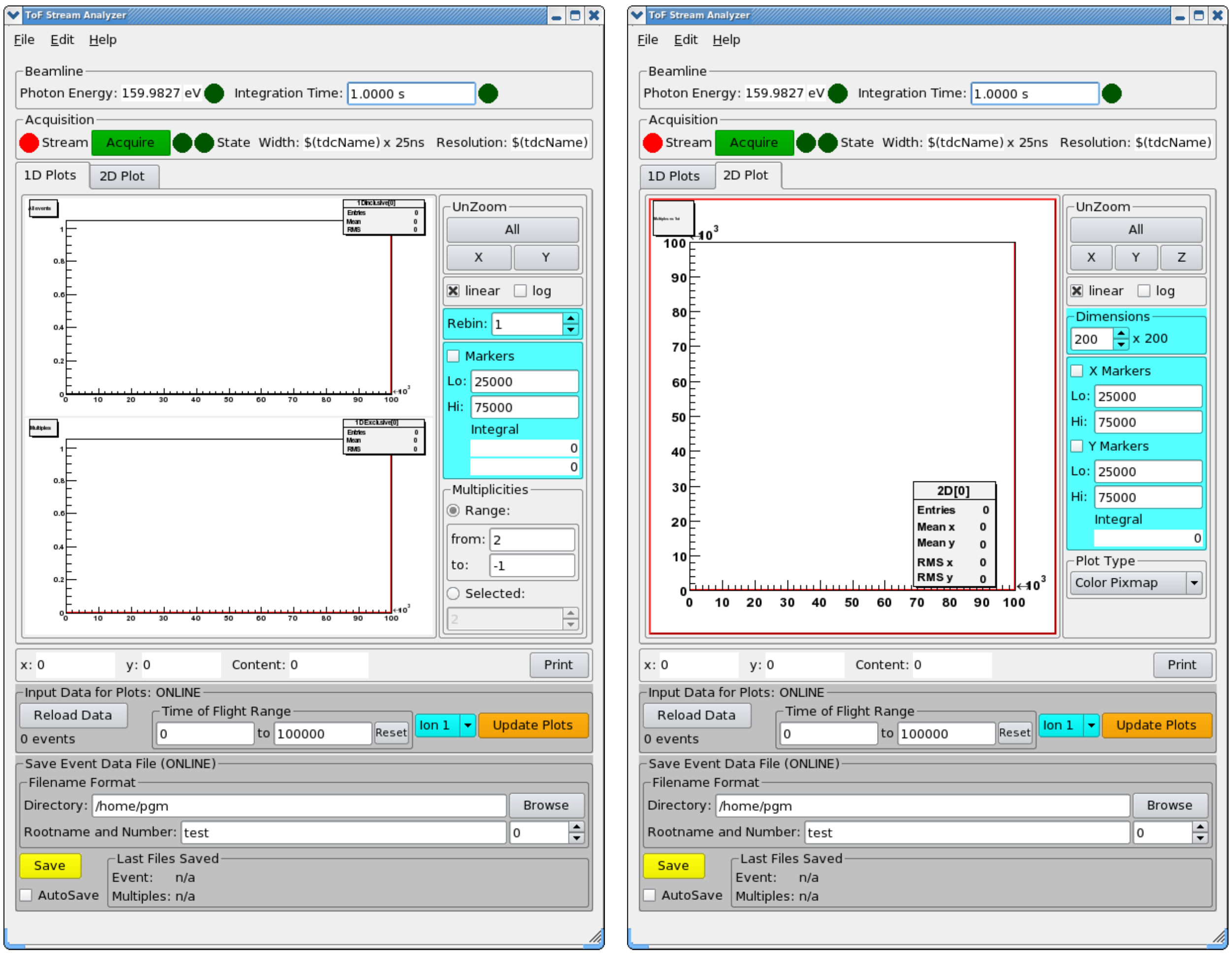


Figure 8. “The ToF Stream Analyser” window showing both the 1D and 2D plot tabs.

The procedure for collecting single multicoincidence spectra is as follows

- Set the required photon energy and beamline and filter conditions, using the “PGM Control Panel” GUI as described in the USERS Manual.
- Check that the “Multihit TDC” GUI is open (figure 7)
- Double click on “New Preview ToF Stream Desktop” icon in the “Time of Flight” folder (figure 3)
- Set “Event Data” to “ASCII Stream” in the “Time of Flight Controls” window (figure 3)
- In “ToF Stream Analyzer” window (figure 6) click “Acquire” until the two green LED icons, to the left of the “Acquire” button, turn on.
    - Click on the orange “Update Plot button” (RHS on lower half of screen)

- If there is an MCA spectrum accumulating in the 1D data window then all is well
    - Click Acquire again and the two green LED icons will turn off
- In the “Time of Flight Controls” GUI (figure 4) set the integration time
- In “ToF Stream Analyzer” window (figure 6) click “Acquire” (Both green LED icons will turn on)
- At this point one can examine the data in the 1D plot tab or 2D plot tab as required. Click “Update Plots” as required. Rescale and rebin as required to analyze the data.
- When satisfied that the data collection is complete and both green LED icons are off click “Update Plots”
- Set the directory path by clicking on the “Browse” button in the “ToF Stream Analyzer” (figure 6)
- Set the rootfile name and index number
- Click “Save” button
- When completely finished with the “ToF Stream Analyzer” window (figure 6) close the window.
- In the “Time of Flight Controls” GUI (figure 4) set “Event Data” to “ No Stream”

4.3.1 File structure of multicoincidence files

When saving data in the “ToF Stream Analyser” several files may be produced. These can be large.

Rootfilename0001.event: This contains an ordered list of all the coincidences recorded and its structure is given below.

```
#text
44 0 33371
44 12 0
45 0 17706
45 12 0
46 0 3364
46 4 3379
46 0 24887
46 12 0
47 0 17949
47 4 21492
47 12 0
48 4 35432
48 12 0
49 0 20888
49 12 0
…
106 0 21364
106 12 0
107 0 36862
107 12 0
109 4 21909
109 12 0
110 0 1811
110 4 1782
110 12 0
…
```

The structure is
Column1 is the number of the electron start event
Column 2 is the channel of the event. (0= Ion channel 1, 4=Ion channel 1, 12=electron)
Column 3 is the time of the event w.r.t. the electron start.
Each event always end with “event number” 12 0.

Rootfilename0001_00.multi: This contains an ordered list of all the coincidences recorded for channel 00 (Ion 1) and its structure is given below. A similar file for 04 (Ion 2) may be produced. Essentially it is a simplified version of Rootfilename0001.event with data only corresponding to one channel.

```
# Ion Times versus Electron Chronology for all multiplicities:
# Incident Energy: 109.999
# Scalers (ion, electron) = 10378 18383
# format:
# - each row corresponds to one electron, which
#   defines the start of a coincidence window.
# - each value (column) across a row corresponds to
#   an ion within the electron coincidence window.
# - rows appear in the order that electrons arrive.
# - ion times are relative to electron start.
33371
17706
3364 24887
17949
20888
3345
21515
33251
21311
27410
18003
30122
18098
19538
3302
24889
```

…

The data columns list all the events (in channel 00) that correspond to Ion 1 stops of an electron. The order of the list is the order in which the events occurred. When two or more numbers are displayed in the same line this is a coincidence event.

Rootfilename0001_00.Excl: This contains an ordered list of all the multi-coincidences recorded for channel 00 (Ion 1) and its structure is given below. A similar file (01) for channel 04 (ion 2) may be produced. Essentially it is a simplified version of Rootfilename0001.multi with data only corresponding to multi-coincidences.

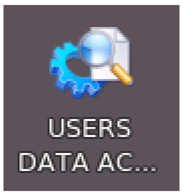
```
# Ion Times versus Electron Chronology for multiplicities 2 and higher:
# Incident Energy: 109.999
# Scalers (ion, electron) = 10378 18383
# format:
# - each row corresponds to one electron, which
#   defines the start of a coincidence window.
# - each value (column) across a row corresponds to
#   an ion within the electron coincidence window.
# - rows appear in the order that electrons arrive.
# - ion times are relative to electron start.
3364 24887
21705 28982
17533 21928
21702 24909
25409 38157
17684 20962
9175 23219
8248 21762
3321 27215
8859 17527
21709 26746
14687 37498
3421 20932
12973 24447
…
30117 33489
3821 16071
27394 33458
15684 26152 29740
3739 8577
21055 24627
13327 15962 25956
17665 21440
13450 15856
17619 27597
…
```

The data columns list all the events (in channel 00) that correspond to two or more Ion 1 stops of an electron. The order of the list is the order in which the events occurred. Column 1 corresponds to the first ion stop in a (multi) coincidence event, column 2 corresponds to the time of the second ion stop in a (multi) coincidence event, column 3 (if it exists) corresponds to the time of the third event in a triple coincidence event etc.

4.4 Recording Partial Ion Yield spectra as a function of photon energy

This section should be read along with the beamline Users Manual.
(http://exshare.lightsource.ca/vlspgm/Pages/Manuals.aspx)
It allows for the collection of complete ToF mass spectra as a function of photon energy. It can also record counts within various ROIs in those mass spectra. Photon Flux, Ring Current and gas pressure are also recorded.

The data acquisition is started by clicking the "Users Data Acquisition" icon on the home screen on the beamline computer.



Referring to the beamline Users Manual: USERS DATA ACQUISITION chapter, the procedure to collect Partial Ion Yield spectra is as follows.

- In the "Data Acquisition Window" opened by double clicking the "Users Data Acquisition" icon
  - Click File → Load
  - Follow directories to "Desktop/User/Gas Phase Configurations"
  - Open file "ToF_Energy Scan_Users_2015"
- Click Graphics → Start_Root_Monitor
  - In "BL Graph" dialog box click "Configure"
  - In "Scan Command" select ".x_.TOF.c"
  - Click Close
  - Do NOT click "Quit" in "BLGraph". Keep the "BLGraph" window open.
- In the "Data Acquisition" window "Control" tab
  - Set the file directory by clicking browse
  - Set the desired filename. Rootfile_%d.dat. The %d allows for the index number to be incremented and appended to the rootfile name.
- In the "Data Acquisition" window "Scan" tab
  - Select the Start value (the largest photon energy required)
  - Select the Delta value (this should be negative)
  - Select the Stop value (this should be the smallest photon energy required)
- In the "Time of Flight Controls" window select the integration time
- In the "Data Acquisition Control" window click "Start"

4.4.1 File structure of Partial Ion Yield files

Recording Partial Ion yield spectra creates two files.

Rootfilename_001.dat: This contains the ancillary data for the Partial Ion Yield spectra. i.e. all the data except the mass spectra themselves. The file structure is a series of comment lines (starting with "#") describing the process variable recorded, followed by data lines in comma separated values (CSV) format. The CSV lines give the photon energy, Kiethly picoammeter currents, ring current, pressure, total electron counts, total ion counts, ROI values and other useful parameters. The meaning of the process variable there are described below.

```
# CLS Data Acquisition
# COMMENT
# END COMMENT
# Event: output
# ID: 1
# column 1: Event-ID
# column 2:  BL1611-ID-2:Energy:fbk NO CONNECTION
# column 3:  A1611-4-11:nA:fbk NO CONNECTION
# column 4:  A1611-4-09:nA:fbk NO CONNECTION
# column 5:  A1611-4-08:nA:fbk NO CONNECTION
# column 6:  A1611-4-02:nA:fbk NO CONNECTION
# column 7:  A1611-4-03:nA:fbk NO CONNECTION
# column 8:  A1611-4-12:nA:fbk NO CONNECTION
# column 9:  BL1611-ID-2:mcs00:fbk NO CONNECTION
# column 10:  BL1611-ID-2:mcs01:fbk NO CONNECTION
# column 11:  BL1611-ID-2:mcs03:fbk NO CONNECTION
# column 12:  TDC1611-I20-01:m13:c00:ROI0
# column 13:  TDC1611-I20-01:m13:c00:ROI1
# column 14:  TDC1611-I20-01:m13:c00:ROI2
# column 15:  TDC1611-I20-01:m13:c00:ROI3
# column 16:  TDC1611-I20-01:m13:c00:ROI4
# column 17:  TDC1611-I20-01:m13:c00:ROI5
# column 18:  TDC1611-I20-01:m13:c00:ROI6
# column 19:  TDC1611-I20-01:m13:c00:ROI7
# not recorded: TDC1611-I20-01:m13:c00:ROI8
# not recorded: TDC1611-I20-01:m13:c00:ROI9
# not recorded: TDC1611-I20-01:m13:c00:ROI10
# not recorded: TDC1611-I20-01:m13:c00:ROI11
# not recorded: TDC1611-I20-01:m13:c00:ROI12
# not recorded: TDC1611-I20-01:m13:c00:ROI13
# not recorded: TDC1611-I20-01:m13:c00:ROI14
# not recorded: TDC1611-I20-01:m13:c00:ROI15
# column 20:  TDC1611-I20-01:m13:c03:ROI0
# column 21:  CCG1611-4-I21-04:vac:p
# column 22:  CCG1611-4-I21-05:vac:p
# column 23:  PCT1402-01:mA:fbk
# column 24:  UND1411-02:gap:mm:fbk
# column 25:  SMTR16114I2004:enc:fbk
# column 26:  TDC1611-I20-01:m13:Histogram_0
# column 27:  TDC1611-I20-01:m13:Histogram_1
#(1)    "Event-ID"     "BL1611-ID-2:Energy:fbk"      "A1611-4-11:nA:fbk"    "A1611-4-09:nA:fbk"
        "A1611-4-08:nA:fbk"    "A1611-4-02:nA:fbk"    "A1611-4-03:nA:fbk"    "A1611-4-12:nA:fbk"
        "BL1611-ID-2:mcs00:fbk"       "BL1611-ID-2:mcs01:fbk"       "BL1611-ID-2:mcs03:fbk"
        "TDC1611-I20-01:m13:c00:ROI0" "TDC1611-I20-01:m13:c00:ROI1" "TDC1611-I20-01:m13:c00:ROI2"
        "TDC1611-I20-01:m13:c00:ROI3" "TDC1611-I20-01:m13:c00:ROI4" "TDC1611-I20-01:m13:c00:ROI5"
        "TDC1611-I20-01:m13:c00:ROI6" "TDC1611-I20-01:m13:c00:ROI7" "TDC1611-I20-01:m13:c03:ROI0"
# Event: background
# ID: 2
# column 1: Event-ID
# column 2:  PGM_mono:selA NO CONNECTION
# column 3:  PGM_mono:Recalib NO CONNECTION
# column 4:  A1611I2:dwell NO CONNECTION
# column 5:  TDC1611-I20-01:m13:UnPairedResolution NO CONNECTION
```

```
# column 6:  TDC1611-I20-01:m13:WindowWidth:fbk NO CONNECTION
# column 7:  TDC1611-I20-01:m13:WindowOffset:fbk NO CONNECTION
# column 8:  TDC1611-I20-01:m13:IntTime NO CONNECTION
# column 9:  PS1611401:400:v0set NO CONNECTION
# column 10:  PS1611401:401:v0set NO CONNECTION
# column 11:  PS1611401:402:v0set NO CONNECTION
# column 12:  PS1611401:403:v0set
# column 13:  PS1611401:404:v0set
# column 14:  PS1611401:405:v0set
# column 15:  PS1611401:406:v0set
# column 16:  PS1611401:200:v0set
# column 17:  PS1611401:201:v0set
# column 18:  PS1611401:202:v0set
#(2)    "Event-ID"     "PGM_mono:selA"       "PGM_mono:Recalib"     "A1611I2:dwell"
        "TDC1611-I20-01:m13:UnPairedResolution"      "TDC1611-I20-01:m13:WindowWidth:fbk"
        "TDC1611-I20-01:m13:WindowOffset:fbk" "TDC1611-I20-01:m13:IntTime"  "PS1611401:400:v0set"
        "PS1611401:401:v0set"  "PS1611401:402:v0set"  "PS1611401:403:v0set"  "PS1611401:404:v0set"
        "PS1611401:405:v0set"  "PS1611401:406:v0set"  "PS1611401:200:v0set"  "PS1611401:201:v0set"
        "PS1611401:202:v0set"
# 2, M3 Angle=0.209614, M3 Angle Correction=-0.000533271, Ammeter integration time=60, TDC bin
width=2, TDC bin width=200, TDC bin width=-195, TDC integration time=600, Ions HV: 3830, 3930.00,
2200.00, 1000.00, 0.00, 3930.00, 1680.00, Electrons HV: 80, 0.00, 0.00
1, 72.0016, 0.0000308, 1.3084670, 0.0000111, 135.9613000, 102.8709000, 0.6196477, 1642519.00,
…1914727.00, 3244534.00, 0, 0, 0, 0, 0, 0, 0, 0, 8089776, 0.0000000185, 0.0000000003, 173.360078,
…98.7537, 160836, 6, 201076
1, 71.5008, 0.0000367, 1.3129000, 0.0000162, 135.0484000, 102.1708000, 0.6177158, 1658223.00,
…1932312.00, 3276815.00, 0, 0, 0, 0, 0, 0, 0, 0, 8179937, 0.0000000184, 0.0000000003, 172.378419,
…98.5329, 157812, 404140, 605344
1, 70.9996, 0.0000364, 1.3113910, 0.0000196, 134.2539000, 101.5405000, 0.6159101, 1666208.00,
…1938715.00, 3288092.00, 0, 0, 0, 0, 0, 0, 0, 0, 8194685, 0.0000000184, 0.0000000003, 171.414830,
…98.3134, 154743, 808572, 1009797
1, 70.4997, 0.0000362, 1.3068300, 0.0000152, 133.5466000, 101.0576000, 0.6141834, 1663771.00,
…1940421.00, 3292867.00, 0, 0, 0, 0, 0, 0, 0, 0, 8126041, 0.0000000184, 0.0000000003, 170.461124,
…98.0914, 151638, 1212980, 1414098
1, 69.9998, 0.0000335, 1.3004600, 0.0000184, 132.8488000, 100.4250000, 0.6123916, 1663585.00,
…1937461.00, 3298689.00, 0, 0, 0, 0, 0, 0, 0, 0, 8094326, 0.0000000185, 0.0000000003, 169.513009,
…97.8743, 148489, 1617129, 1818183
1, 69.4998, 0.0000401, 1.2934230, 0.0000234, 132.1971000, 99.9984900, 0.6107854, 1661621.00,
…1934849.00, 3303191.00, 0, 0, 0, 0, 0, 0, 0, 0, 8064870, 0.0000000185, 0.0000000003, 168.575377,
…97.6523, 145294, 2021206, 2222214
………
```

The ellipses (…) above are not recoded in the file itself. They indicate that the line is a continuation of the line above, and in the last instance that there is more data in the file.

Rootfilename_001_spectra.dat: This contains in each row the complete Time of Flight histogram (In CSV format) corresponding to each CSV line in the file Rootfilename_001.dat. This file can be unwieldy as it is typical for the mass spectrum – a histogram of counts in each time bin in ToF spectrum – to have up to 50,000 bins for each of ion channel 1 and ion channel 2. If both ion channels are recorded that amounts to 100,000 columns in each row of the file. This is more than can easily be opened by many common programs (e.g. Excel).

Process Variable Name	Description
Event-ID	States which data are being recorded as described in the header
BL1611-ID-2:Energy:fbk	Monochromator Energy (eV)
A1611-4-11:nA:fbk	Endstation Photodiode Current (nA)
A1611-4-09:nA:fbk	Total Electron Yield Current(nA) not connected to the ToF apparatus
A1611-4-08:nA:fbk	Total Fluorescent Yield Current (nA) not connected to the ToF apparatus
A1611-4-02:nA:fbk	Branch A Exit Slit Lower Blade Current (nA)
A1611-4-03:nA:fbk	Branch A Exit Slit Upper Blade Current (nA)
A1611-4-12:nA:fbk	Beamline Ni Mesh Io current (nA)
BL1611-ID-2:mcs00:fbk	Total Electron Counts
BL1611-ID-2:mcs01:fbk	Total Ion 1 Counts
BL1611-ID-2:mcs03:fbk	Total Ion 2 Counts
TDC1611-I20-01:m13:c00:ROI0	Total Counts ROI 0 – Ion 1
TDC1611-I20-01:m13:c00:ROI1	Total Counts ROI 1 – Ion 1
TDC1611-I20-01:m13:c00:ROI2	Total Counts ROI 2 – Ion 1
TDC1611-I20-01:m13:c00:ROI3	Total Counts ROI 3 – Ion 1
TDC1611-I20-01:m13:c00:ROI4	Total Counts ROI 4 – Ion 1
TDC1611-I20-01:m13:c00:ROI5	Total Counts ROI 5 – Ion 1
TDC1611-I20-01:m13:c00:ROI6	Total Counts ROI 6 – Ion 1
TDC1611-I20-01:m13:c00:ROI7	Total Counts ROI 7 – Ion 1
TDC1611-I20-01:m13:c03:ROI0	Total Counts ROI 0 – electrons
CCG1611-4-I21-04:vac:p	Pressure Time of Flight Section (Torr)
CCG1611-4-I21-05:vac:p	Pressure Differential Section (Torr)
PCT1402-01:mA:fbk	Ring Current (mA)
UND1411-02:gap:mm:fbk	Undulator Gap (mm)
SMTR16114I2004:enc:fbk	Monochromator encoder feedback
TDC1611-I20-01:m13:Histogram_0	Internal MCA Histogram Structure
TDC1611-I20-01:m13:Histogram_1	Internal MCA Histogram Structure

Table 3. The process variables recorded in the CSV section of a Partial Ion Yield dataset.

4.5 Recording Partial Ion Yield spectra as a function of photon energy with streaming.

It is also possible to record muticoincidence spectra as a function of photon energy. This allows the production of an ordered stack of PEPICO maps. The procedure for this is as follow

- In “Time of Flight Controls” GUI
    - Set Event data as “ASCII Stream”
    - Click “Stream Analyzer”
- In “Stream Analyzer” window
    - Click on “Browse” and set the directory
    - Set the rootfile name
    - Set the starting sequence number
    - Check the “AutoSave” button to be on. (checkmark visible)
- Set up the scan parameters in “Beamline Data Acquisition” window
- Set the collection time in the “Main Beamline Control” and “Time of Flight Controls” windows
- In “Multihit TDC GUI” window ensure that the ToF Engine is “Stopped”
- In “Beamline Data Acquisition” wind click on start

4.5.1 File structure of multicoincidence files recorded against photon energy

In addition to creating the Partial Ion Yield Files recorded above (3.3.1), this mode records the multicoincidence files (3.2.1). With the multicoincidence files the file index numbers increases by one for each photon energy recorded.

5. *Typical results*

A mass spectrum of Argon (Ar) excited at 110eV photon energy is presented.

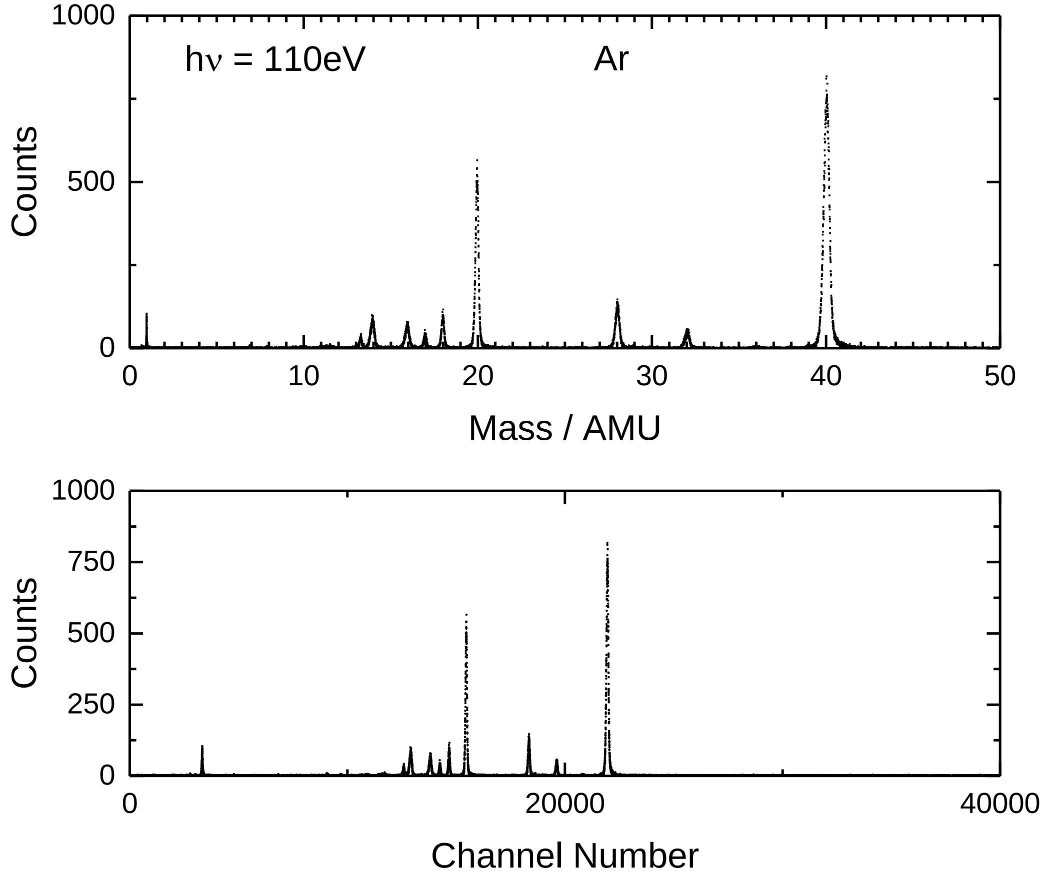


Figure 9 Photoionization mass spectrum of Argon recorded at 110eV photon energy

Ion MCP Grid	-3830 V	Electron MCP Bias	240 V
Ion Drift Tube	-3930 V	Front Electron Mesh	2060 V
Ion Lens	-2600 V	Electron G2, G3	200 V
Front Ion Mesh	-1600V		
Ion MCP Front	-3930 V		
Ion MCP Back	-1730 V		

Table 4 the voltage settings used to create figure 9

A mass spectrum of Toluene ($C_6H_5CH_3$) excited at 100eV photon energy is presented.

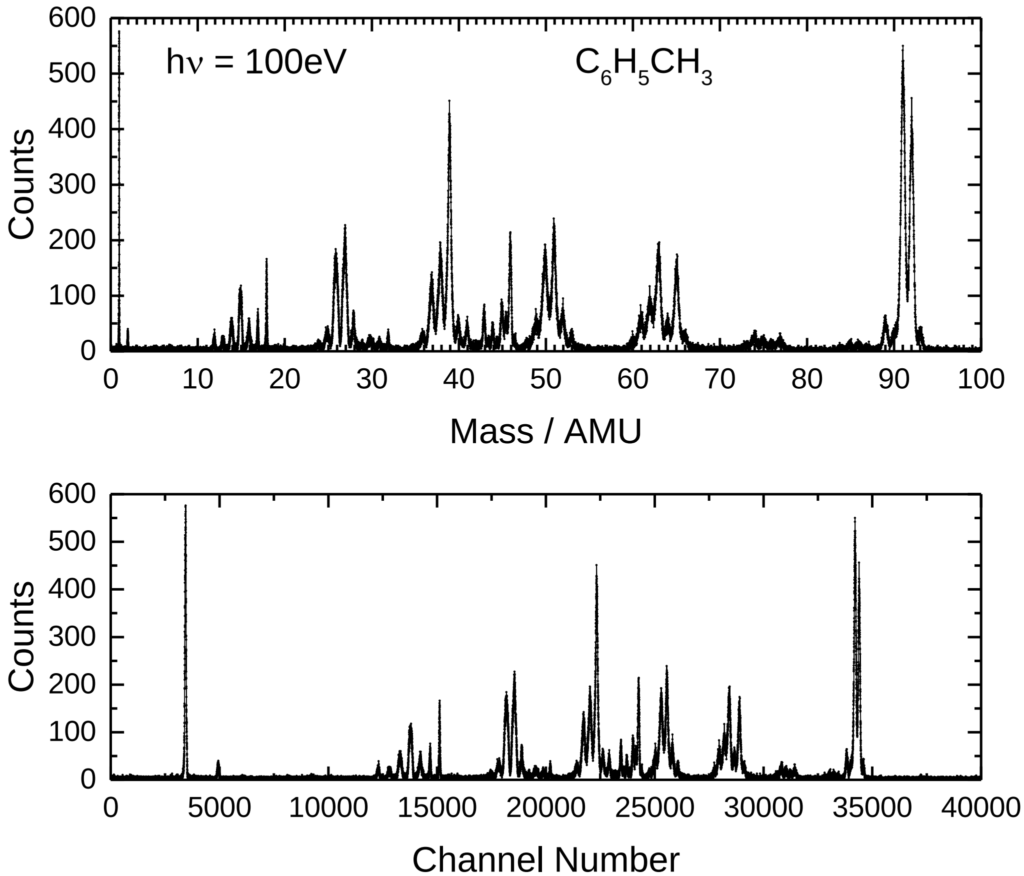


Figure 10 Photoionization mass spectrum of Toluene recorded at 100eV photon energy

Ion MCP Grid	-3830 V	Electron MCP Bias	2450 V
Ion Drift Tube	-3930 V	Front Electron Mesh	1276 V
Ion Lens	-2200 V	Electron G2, G3	200 V
Front Ion Mesh	-1000 V		
Ion MCP Front	-3930 V		
Ion MCP Back	-1680 V		

Table 5 the voltage settings used to create figure 10

6. *Connecting the High Voltages*

The high voltages for the Time of Flight are supplied by the CAEN SY2527 Universal Multi-channel Power Supply System via a patch panel located above the beamline.

Figure 11 The High Voltage patch panel.

The table below shows the how the channels for the patch panel correspond to the voltages required.

Channel	**Corresponding Voltage**	**Attaches to**
1+	G 2-3	Electron Box
3+	E MCP Bias	Electron Box
11+	Front Electron Mesh	Electron Box
0-	MCP Grid	Mini-Conflat Cross
1-	Drift Tube	Mini-Conflat Cross
2-	Lens	Mini-Conflat Cross
3-	Front Ion Mesh	Mini-Conflat Cross
4-	Ground	Do Not Connect
5-	Ion MCP Front	Ion Box
6-	Ion MCP Back	Ion Box

Table 6 Voltages supplied by the patch panel

The voltages are connect to the instrument at three locations. A six way miniconflat cross at the top of the apparatus, an electron voltage divider and pre-amplifier box and an ion voltage divider and pre amplifier box.

There are two SHV connections that should be shorted to ground. The Ion Ground on the mini-conflat cross and the electron float on the electron box.

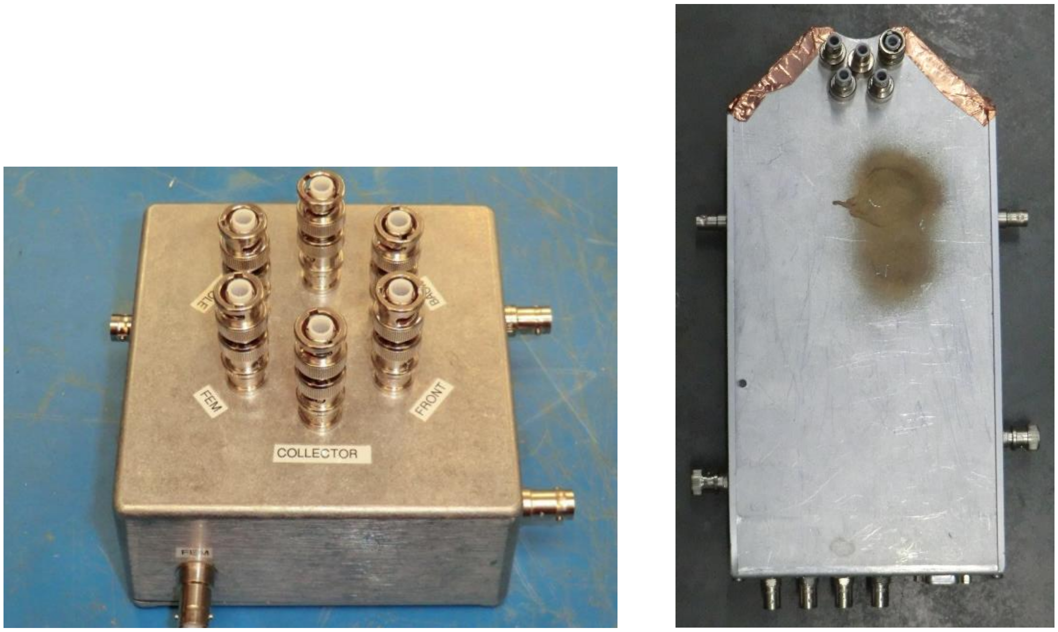


Figure 12 Electron (left) and Ion (right) voltage divider and preamplifier boxes.

The electron box attaches to the apparatus at the feedthrough conflat at the bottom of the Time of Flight section. Take care to match the feedthrough when attaching the electron box as it is possible to connect the box in different orientations. The ion box attaches to the feedthroughs next to the mini-conflat cross at the top of the Time of Flight section.

7. *Signal Processing and Connections*

There are three main sections to the signal processing system: the ion and electron voltage divider and pre-amplifier boxes, the NIM crate and units on the lower shelf of the instrument table and the VME half rack.

The signals from the electron and ion MCPs are fed to the electron and ion voltage divider and pre-amplifier boxes. These need power to operate. This is supplied from a unit in the NIM crate. The output from the pre-amplifiers is sent to the Tennelec Quad Constant Fraction Discriminator (CFD). Outputs from the CFD are fed to ratemeters, an oscilloscope and the VME half Rack. It is in the VME half rack that most of the signal processing takes place. It contains both a NIM bin and VME crate.

The Instrument NIM bin requires the following units

- Tennelec TC454 Quad Constant Fraction Discriminator (CFD)
- CLS 15V dual power supply (PS)
- 3x Ortec 661 Ratemeter

The VME half rack NIM bin requires the following units

- Caen N454 4-8 logic Fan-in-Fan-out (FIFO)
- Caen N89 NIM-TTL Adaptor (NTA)
- Caen N385 3 fold logic unit (LU)
- Caen N93B dual timer (DT)

The VME half rack VME create requires the following units

- Caen V1290N 16CH 25ps Multihit TDC (TDC)
- SIS GmbH SIS36/38xx Scaler (Sc)
- SIS GmbH SIS3100 Gigabit Crate Controller optical link (C)

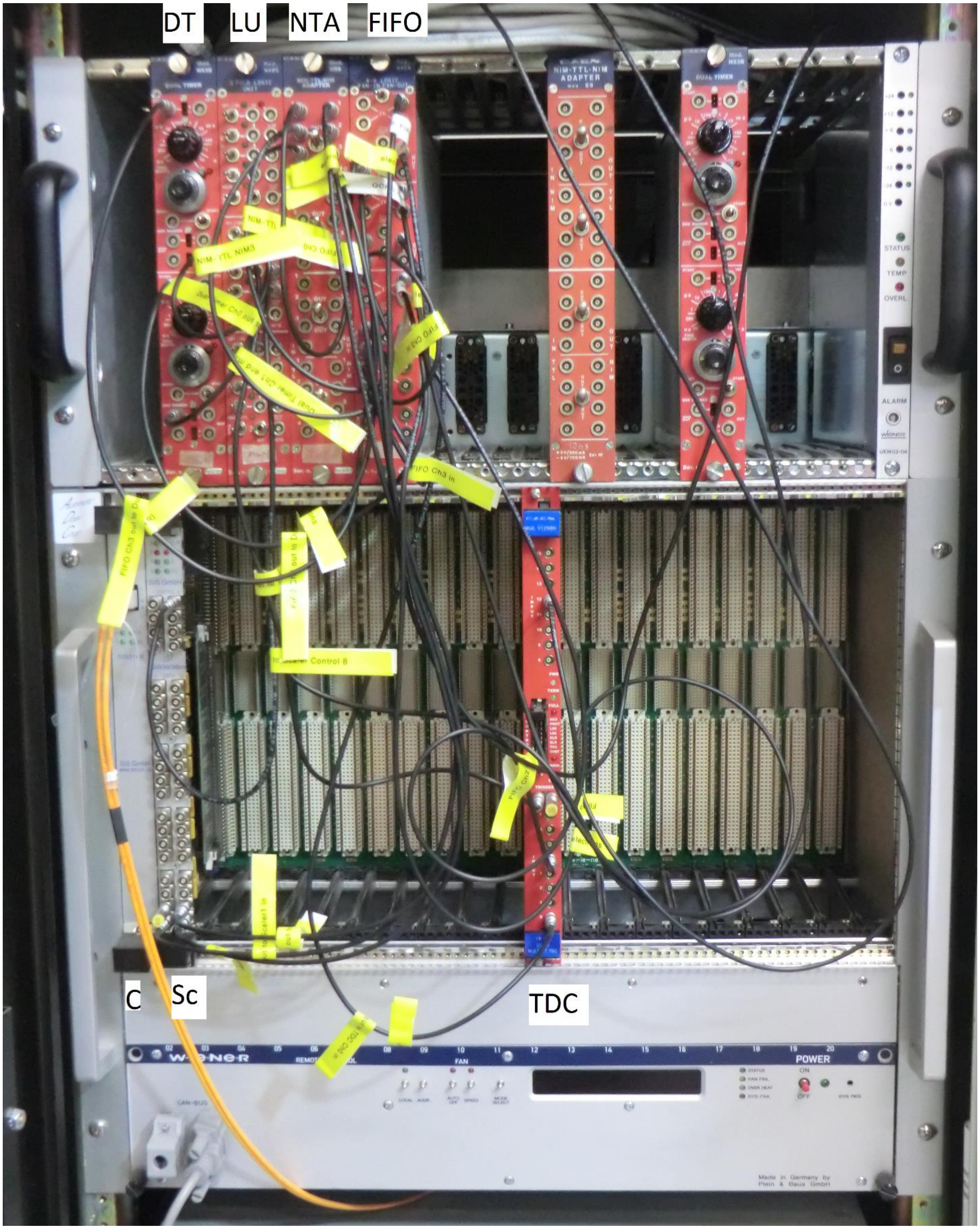


Figure 13 NIM and VME units in the data acquisition half rack

The table below gives the Lemo connections required process the signals properly. The connections are usually left in place. The only exception are the three connections between the Instrument NIM bin and the VME half rack.

Electron Chain		**Ion 1 Chain**		**Ion 2 Chain**	
Connects from	Connects to	Connects from	Connects to	Connects from	Connects to
15V PS Out	15V PS in electron box	15V PS Out	15V PS in Ion box.		
Preamp Out (Electron)	CFD Ch2 in	Preamp Out (Ion 1)	CFD Ch0 in	Preamp Out (Ion 2)	CFD Ch1 in
CFD Ch2 Delay out	CFD Ch2 Delay in	CFD Ch0 Delay Out	CFD Ch0 Delay In	CFD Ch1 Delay Out	CFD Ch1 Delay in
CFD Ch2 Out	E- Ratemeter (Neg in)	CFD Ch0 Out	Ion 1 Ratemeter (Neg in)	CFD CH1 Out	Ion 2 Ratemeter (Neg in)
CFD Ch2 Out	Scope (optional)	CFD Ch0 Out	Scope (optional)	CFD Ch1 Out	Scope (optional)
CFD Ch2 Out	FIFO in Ch0	CFD Ch0 Out	FIFO in Ch1	CFD Ch1 Out	FIFO in Ch 2
FIFO Out Ch0	TDC in Ch12	FIFO Out Ch1	TDC in Ch0	FIFO Out Ch2	TDC in Ch4
FIFO Out Ch0	NTA NIM in Ch1 (toggle=out, up)	FIFO Out Ch1	NTA NIM in Ch2 (toggle=out, up)	FIFO Out Ch2	NTA NIM in Ch2 (toggle=out, up)
NTA TTL Out Ch1 (toggle=out, up)	Scaler Ch4	NTA TTL Out Ch2 (toggle=out, up)	Scaler Ch2	NTA TTL Out Ch3 (toggle=out, up)	Scaler Ch1
FIFO Out Ch0	DT Start Ch1	FIFO Out Ch1	FIFO in Ch3	FIFO Out Ch2	FIFO in Ch3
		FIFO Out Ch3	DT Start Ch0		
DT Endmarker Ch1	LU in Ch2 (toggle on) (Majority AND)	DT Out Ch0	LU in Ch2 (toggle on) (Majority AND)		
LU out Ch2 (toggle off) (Majority AND)	TDC Trigger	LU out Ch2 (toggle off) (Majority AND)	Scaler Control Ch8		
TDC Trigger	50 Ohm terminator	Scaler Ch3	50 Ohm terminator		
SIS optical Link	PC optical Link				

Table 7 Signal processing chain connections

8. Behind the scenes settings

In the configuration tab of the multihit TDC Gui (figure 5) the following settings should be made. Ch0, Ch4 and Ch12 should be enabled, the rest should be disabled. The setpoint and offset should be given as in table 5. The unpaired resolution is 100ps

The potentiometers on the Dual Timer (see figure 13) should be set at in table 4.

	Setpoint	Offset	Dual Timer Ch0 Pulse stretcher	Dual Timer Ch1 Trigger delay
Light Molecule	200	-195	0-5µs (3.1 on Dial)	0-4µs (2.4 on Dial)
Heavy Molecule	400	-395	0-9.8µs (7.05 on Dial)	0-9µs (6.30 on Dial)

Table 8 Setpoint, Offset and Dual Timer settings.

Typical settings for the CFDs are: Threshold = - 0.5V, Z = -0.021V, W = 150ns (max)

On the configuration tab of the Multihit TDC Gui (Figure 7) click on the Configuration tab Then change the setpoint and width.

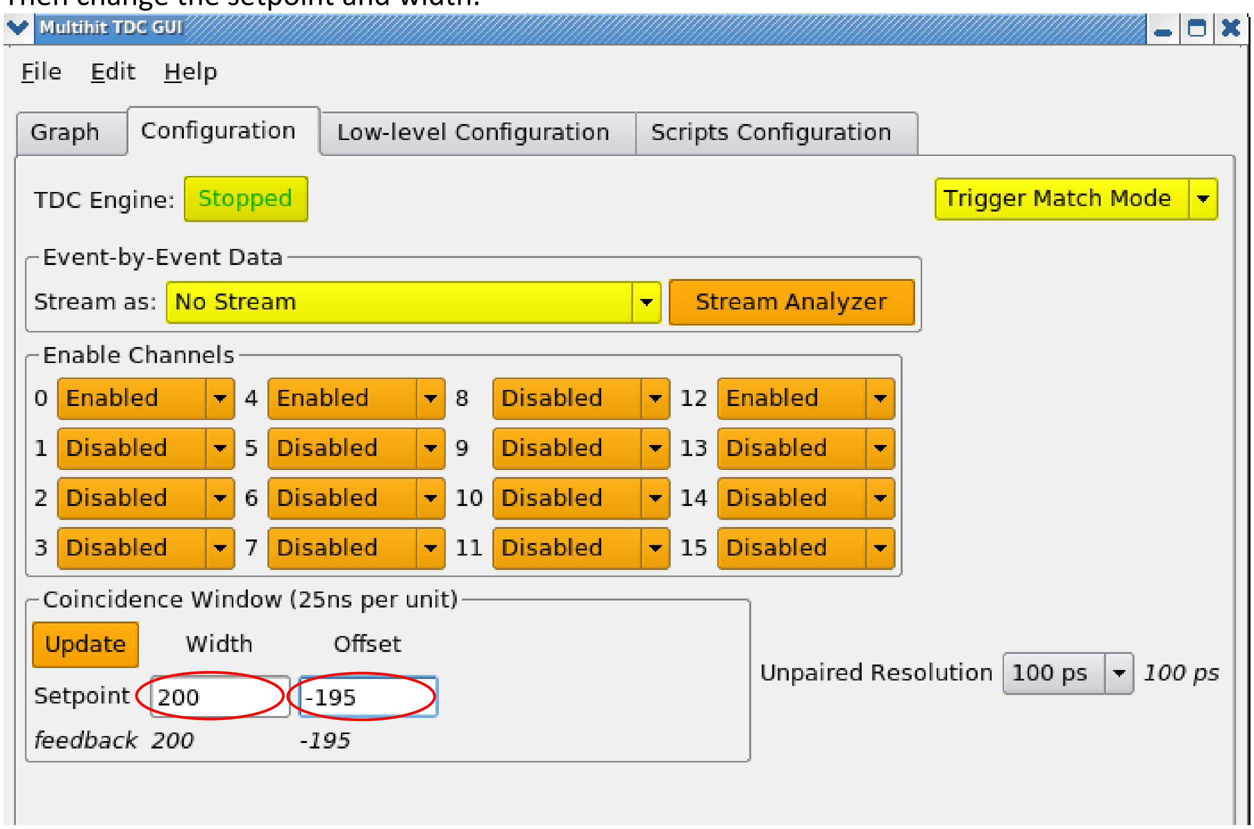


Figure 14 Changing the setpoint and width on the ToF Configuration GUI

9. *References*

[1] W.C. Wiley, I.H. McLaren, Time-of-Flight Mass Spectrometer with Improved Resolution, Review of Scientific Instruments, 26 (1955) 1150-1157.

[2] A.C. Guerra, J.B. Maciel, C.C. Turci, R.C. Bilodeau, A.P. Hitchcock, Quantitative oscillator strengths for ionic fragmentation of C 1s and O 1s excited CO, Canadian Journal of Chemistry, 82 (2004) 1052-1060.