ASTON IMPACT SOFTWARE MANUAL

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Revision History

Revision	ECO	Change Log	Author
A	ECO-001XX	No Content Changes	Vinay Kulkarni

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1. USER INTERFACE

The user interface is one of the primary modes of communicating with Aston Impact and acquiring analytical data out of it. AtonLab provides customizability and exposes many configuration parameters that govern the behavior of the system.

1.1 Client system requirements

The minimum and recommended client PC requirements for running the Aston UI application are provided below

Table 11. System requirement

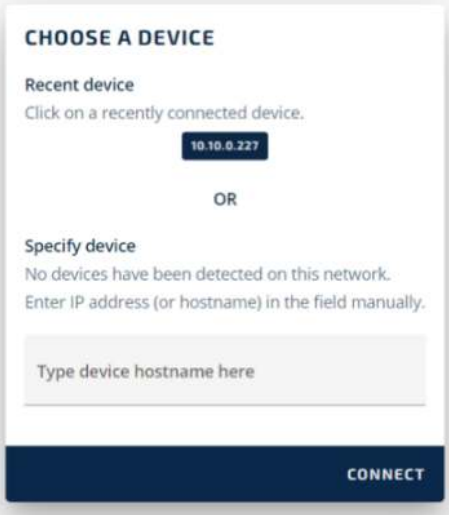
REQUIREMENTS	RECOMMENDED
Processor	Core i5 or higher AMD A8 or higher Mac model year 2014 or later
System Memory	16 GB or higher
Graphics	Intel HD Graphics, AMD APU graphics, NVIDIA GeForce or AMD Radeon GPUs
Primary Storage	1 TB SSD
Operating system	Windows 10, MAC operating system-X 10.10 (Yosemite) or higher , Ubuntu 20.04
Network	1 Gbps
Display resolution	1920 x 1080 or higher

1.2 Accessing the UI Client

The Aston Impact system is accessed through the Windows Application.
For Installation procedure, please refer to the Install guide section

Steps to open the Application

- Double click on the Aston Impact application icon
- The window when opens up would prompt to choose a device
- Enter the system host name or ip address e.g., test009.atoms.app



1.2.1 User Interface

1.2.1.1 Aston Impact Exclusive Access

Server maintains an (exclusive) session with a user whenever they open the UI in their client application. When there are no sessions reserved by the server, any user who opens the UI in their application will get access right away. Just like usual. If one user is actively using the UI, other users trying to open the UI in their application will not get access right away. Instead, a negotiation will begin. The new user who wants access will see this:

> This device is currently reserved for another connected user.
> They have been requested to transfer control over to you.
> They can either accept or reject the request.
> If they don't respond, control will transfer to you.
> Waiting 48 seconds for their reply

- The user who is already using the UI can either choose to
    - Approve: Session will end, and UI will close. The new user who wanted access will now get an exclusive session, and they can continue to use their UI.
    - Reject: Session will continue as usual. The new user who wanted access will get denied.
- Notice the 30 seconds countdown timer on both screenshots. If the user who is already using the UI does not respond (click either button) before countdown reaches 0 seconds, the new user automatically gets the exclusive session (as if the Approve button had been pressed). This is so that if a user is away from their system and not there to respond, another user on a system somewhere else can still take over the UI access and control the device.
- When any user who has the exclusive session closes the UI (client application), their session will automatically end 60 seconds after the instant they closed the UI. If the active user closes the UI, then re-opens before 60 seconds have passed, they will retain the access and the UI will continue to work as usual.

1.2.1.2. Application Tips

- Closing the application does not end the active session right away. It ends 60 seconds after the instant they closed the UI.
    - Refreshing window can be performed without the risk of losing the session to another user next in line.
    - Accidental closing of the application does not result in losing a session and another user next in line taking over control.
- If two users U1 and U2 want to transfer control, where U1 is in active session:
    - Do not -- U1 closes their application and then U2 opens UI in their application.
        - This will result in U2 unnecessarily having to wait "T" seconds before being granted an active session.
    - Do -- U2 goes ahead and opens UI in their application, then U1 gets the prompt to approve override, U1 approves override, then U2 gets the active session, then U1 closes their application.
        - This will result in U1 quickly getting the active session without any wait period.

1.3 Navigation menu bar

The vertical navigation menu on the left of the user interface provides access to pages that help realize the primary use-cases for the Aston Impact. The system tray at the bottom of the navigation menu bar provides additional system information.

1.3.1 Navigation icons

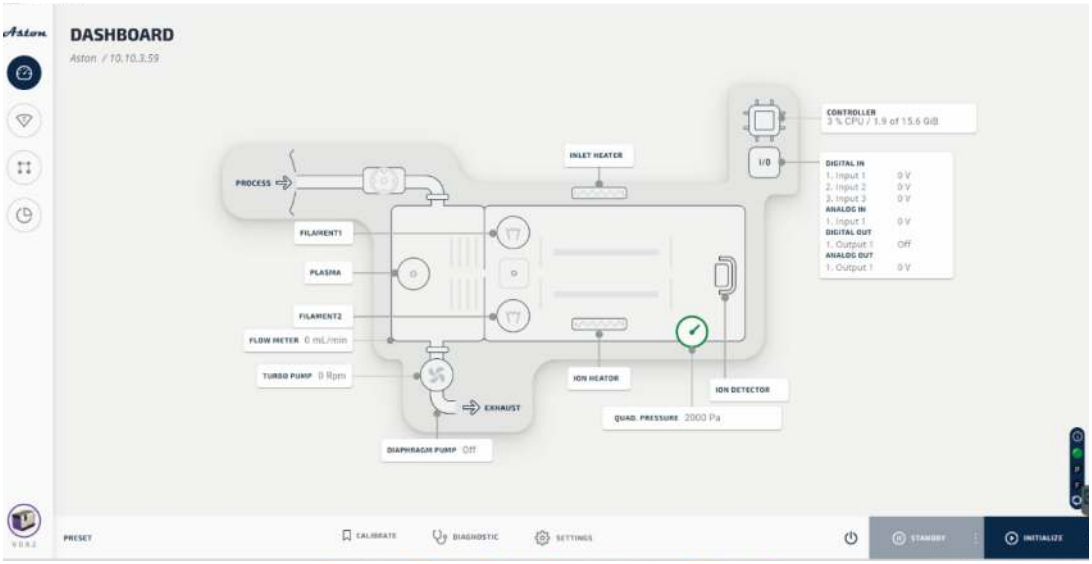
Various pages in the UI to configure and use the system.

Table 12. Navigation icons parameter description

PARAMETER	DESCRIPTION
Dashboard 	The main page of the UI from where data acquisition can be triggered, visualized, and downloaded. The system state can be visualized and controlled from this page. The user can also trigger other features like diagnostics and calibration.
Scan 	The user can configure various data acquisition properties and save them as reusable presets. Users can also trigger scans and visualize the acquired data.
Workflow 	The user can configure complex data acquisition sequences through a visual programming language and save them as reusable presets. Users can also trigger workflows and visualize the acquired data.
Reports 	All data acquired in the system and properties monitored by the system can be downloaded and visualized from this page.

1.4 Dashboard

The dashboard is the primary page for the user to interact and monitor the Aston Impact.



1.4.1 System diagram & controls

The dashboard block diagram indicates the state of the Aston Impact system. Status of the main system components are indicated in panel boxes.

NOTE

The user can edit any component state by clicking on the corresponding component panel or on the component icon to see an expanded list of adjustable settings and read-only values.

Click on the device to see the advanced settings panel for the component.

1.4.1.1 Filament 1 and 2

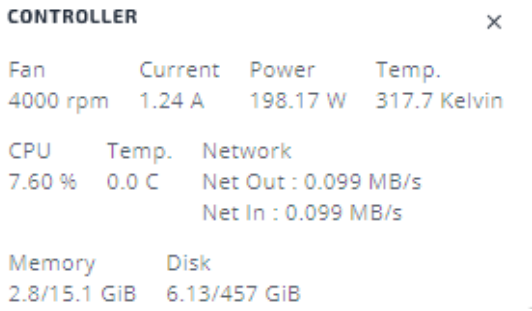
Each filament has a window and associated parameters as shown below.

PARAMETER	DESCRIPTION
Filament current	Current draw for filament producing the emission
Filament voltage	Voltage applied on the filament
Filament power	Power consumed by the filament
Filament resistance	Filament resistance used to indicate health of the filament
Device on/off	Indicates whether filament is on or not
Emission current set point	Requested emission current set point
Emission current live value	Live emission current value

1.4.1.2 Input / Output

Displays analog/digital input or output values. Users can on/off the AUX digital out and can input the values in the AUX analog out manually.

1.4.1.3 Controller

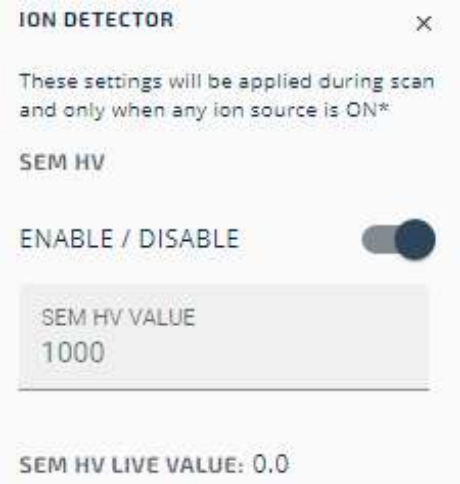


PARAMETER	DESCRIPTION
Controller fan	Controller fan speed
Controller current	Controller current draw
Controller power	Controller power consumption
Controller temperature	Controller temperature
CPU	CPU utilization
CPU temp	CPU temperature
Memory used	RAM usage
Disk used	eMMC Usage
Network	Network throughput (on network controller not connected to PLC)

1.4.1.4 Ion Detector

When SEM HV is set to ENABLE, the SEM voltage is raised to the setpoint (1000 V for instance) automatically when the scan is initiated

When set to DISABLE, the SEM remains OFF.



PARAMETER	DESCRIPTION
SEM HV	Enable/Disable for ion detection

1.4.1.5 Quadrupole pressure

Indicates pressure in the quadrupole chamber in the selected unit (Pa, Torr, etc.)

1.4.1.6 Ion Heater

Users can turn on/off the ion heater and set it to the desired temperature. The recommended setting is 150℃.

1.4.1.7 Turbo Molecular Pump (TMP)

Users can turn on/off the turbo pump. When device is ON, user can change the turbo pump speed (Percentage)

The TMP window includes pump diagnostics such as speed, power, and temperatures of components including motor, bearings, and electronics.

1.4.2 Device state indication

Colored component icons are used to indicate the state of the component.

PARAMETER	DESCRIPTION
On	Green indicates the system component is ON.
Off	Grey indicates the system component is OFF.
Error	Red indicates an error in the system component

1.4.3 Settings

Aston Impact's advanced settings can be customized by the user and saved. Certain settings are password protected and meant only for the internal user. Advanced settings can be viewed by clicking the advanced icon. Each setting is described in the right panel.

1.4.3.1 Vacuum

Table 13. Vacuum parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Pump				
Turbo pump speed set point	Pump speed that needs to be achieved before initialization is considered complete.	20 %	100 %	100 %
Stop scan on poor turbo pump speed control	Stop scan when there is a deviation beyond tolerance from the requested set point.	-	-	Enable
Turbo pump poor speed control tolerance	Tolerance range for Turbo pump speed set point. If pump speed is within the tolerance, no action is taken. If pump speed is beyond the tolerance limit for more than two minutes (configurable with Turbo startup pressure wait time), scans are stopped.	1 %	30 %	10 %
Turbo pump poor speed control recovery wait time	Time for which the system waits for pump RPM to recover within tolerance of pump speed set point. After this time, an error is reported.	0.3 s	600 s	180 s

Safety

Turbo pump startup pressure	Minimum pressure needed in the chamber, after achieving which turbo pump is powered on and set to high RPM.	0 Pa	2666 Pa	1333 Pa
Turbo pump startup pressure wait time	Time at which the turbo pump waits for the chamber pressure to reach startup pressure after which it errors out.	0.3 s	600 s	180 s
Turbo pump auto- power-off pressure	Maximum permitted chamber pressure, which when exceeded the turbo pump is brought to 0 RPM.	0 Pa	1333 Pa	1.3332237 Pa
Power off turbo pump at high power	If the pump power consumption exceeds the safe limit, power off the turbo pump.	-	-	Enable
Turbo pump safe power limit	If the pump power consumption does not fall below this limit within the Turbo pump safe power timeout, then the system is put into standby.	1 Watt	50 Watt	15 Watt
Turbo pump safe power timeout	Time after which if the turbo pump power does not fall below the Turbo pump safe power limit, the system is put into standby.	1 s	1000000 s	3600 s

Pressure

Pressure averaging	Multiple pressure samples are averaged before reporting to eliminate noise in the pressure data	-	-	Disable

1.4.3.2 Filament

Table 14. Filament parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Emission control				
Emission control loop	Emission control loop mode	-	-	Closed loop
Filament type	Filament Material	-	-	Yttria
Filament current trip limit (Yttria)	Maximum permitted drive current for the filament, which when exceeded, the source is shutdown. This is defined by the filament's safety limit specification.	0 A	4.2 A	1.55 A
Filament max supply voltage (Yttria)	Sets the maximum voltage available to drive the filament.	1.4 V	1.9 V	1.7 V
Emission convergence delays (Yttria)	Delay between first convergence to desired emission current and start of control loop.	1 µs	1000000 µs	300000 µs

Emission coarse control tuning constant (Yttria)	Filament voltage coarse tuning constant that determines response and stability of emission control loop.	0	2	0.00016
Emission fine control tuning constant (Yttria)	Filament voltage fine tuning constant that determines response and stability of emission control loop.	0	2	0.06
Filament voltage change delay (Yttria)	Delay between each filament voltage set command until emission current set point is achieved.	1 µs	1000000 µs	300000 µs
Emission current convergence timeout (Yttria)	Maximum amount of time to wait to converge to Emission current. If desired current can't be achieved, a timeout error is reported.	10 ms	5000 ms	3000 ms
Health				
Filament health monitor	Enable or disable filament health monitoring.	-	-	Enable
Unused emission source resistance	Resistance of a good unused filament.	0.1 Ohm	5 Ohm	1 Ohm
Failed emission source resistance	Resistance of a filament at its end of life.	0.1 Ohm	5 Ohm	1.7 Ohm
Filament health rate duration	Rate of change of filament resistance is calculated over this duration.	2 s	3600 s	900 s
Filament health monitoring frequency	Filament health is calculated periodically at this interval.	1 min	180 min	1 min

Table 14. Filament parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Safety				
Filament idle auto-off	Controls whether the filament automatically powers off on idle.			Enable
Filament idle auto-off timeout	Time after which filament is de- energized if no scan is run. Ion Source Lock must be enabled in the UI for this setting to take effect.	5 s	8640000 s	300 s

Filament safe pressure limit	Pressure above which the filament is de-energized. When below threshold, the filament is energized. System enters a standby state if pressure remains above this threshold after Emission safe pressure check timeout.	0.1333~~3224~~ Pa	2.666~~4474~~ Pa	0.666~~6118~~ Pa
Pause scan on filament safe pressure violation	Enable/Disable scan pause when pressure deviates beyond Poor emission control tolerance.			Enable
Filament safe pressure violation ignore duration	Scans are typically paused when Filament safe pressure limit is exceeded. The limit violation can be ignored for this specified duration.	1 s	120 s	15 s
Filament safe pressure check timeout	Timeout duration for checking if pressure has reached below Filament safe pressure limit.	1 s	1800 s	90 s
Emission tolerance for aggressive control	Convergence tolerance for Emission current set point. Within this tolerance, no voltage adjustments are performed. Beyond this tolerance limit, voltage is adjusted but scan continues to run if pressure is between lower and upper limit.	0 %	10 %	0.5 %
Pause scan on poor emission control	Enable/Disable scan pause when emission deviates beyond upper tolerance limit.			Enable
Poor emission control tolerance	If emission current deviates from the set point by this value, the scan is paused, and the system attempts to reconverge. If emission current is within this tolerance value, the system attempts to converge to the emission current set point without pausing the scan.	0 %	1000 %	5 %
Poor emission control scan-pause ignore duration	Scans are typically paused when Poor emission control tolerance is exceeded. The limit violation can be ignored for this specified duration.	1 s	120 s	15 s

1.4.3.3 Mass filter

Table 15. Mass filter parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Mass calibration 3rd order Coefficient	Mass axis errors, if observed, are corrected by changing RF amplitude using a polynomial relationship. New RF = aRFˆ3 + bRFˆ2 + cRF + d. This is the value of 'a'.	-100000 1/amu2	100000 1/amu2	0 1/amu2
Mass Calibration				
Mass calibration 2nd order coefficient	Mass axis errors, if observed, are corrected by changing RF amplitude using a polynomial relationship. New RF = aRFˆ3 + bRFˆ2 + cRF + d. This is the value of 'b'.	-100000 1/amu	100000 1/amu	0 1/amu
Mass calibration slope	Mass axis errors, if observed, are corrected by changing RF amplitude using a polynomial relationship. New RF = aRFˆ3 + bRFˆ2 + cRF + d. This is the value of 'c'.	-100000	100000	1
Mass calibration intercept	Mass axis errors, if observed, are corrected by changing RF amplitude using a polynomial relationship. New RF = aRFˆ3 + bRFˆ2 + cRF + d. This is the value of 'd'.	-100000 amu	100000 amu	0 amu
Others (Note: The password protected fields are only for Atonarp engineers to use.)				
RF frequency search iterations	Number of iterations for RF frequency search execution.	1	100	10
Maximum mass range	The maximum mass that can be scanned.	100 amu	285 amu	250 amu
Transmission mass power	When the Composition estimator model is Simple molecule and sensor model (TR), the measured ion currents are scaled by the transmission of their masses raised to this power.	0	10	1

Quadrupole field radius	Radius of the gap between the quadrupole through which the desired ions traverse to the Faraday cup.	0 m	100 m	0.0013266 m
RF settling time	RF Voltage settling time period.	0 µs	10000 µs	1000 µs
Reference mass to set DC for RF only scan	Mass to be considered for calculating the fixed DC+ and DC- voltage for RF only scan. The DC does not vary with the RF. It is held equivalent to the mass specified.	0 amu	20 amu	1 amu
Zero-blast correction				
Zero-blast correction	The zero-blast signal corresponds to a mass independent signal that floods and overwhelms the detector at lower masses. This is because the RF and DC fields are too low to stop all ions from reaching the detector. The extent of the zero-blast problem depends on the physical dimensions of the filter, the frequency of the RF and the energy of the ions that traverse the length of the quadrupole filter.	-	-	Enable
Zero-blast scan end mass	The upper limit of masses scanned for zero blast correction.	0 amu	7 amu	2 amu
Zero-blast correction end mass	The upper limit of masses till which zero blast curve is extrapolated for correction.	0 amu	7 amu	6 amu
Zero-blast scan step size	The step size with which masses are scanned until Zero-blast scan end mass.	0.1 amu	0.3 amu	0.1 amu
Log ZB pre-correction scan data into reports	Enable/disable the writing of zero blast uncorrected scan data into the report file	-	-	Disable

1.4.3.4 Debug

Table 16. Debug parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Logging				
Debug scan	Enable debug scan mode that produces a more verbose report. This will increase scan time.	-	-	Disable
Log detector ADC raw data	Record ion detector ADC raw data.	-	-	Disable
Log detector ADC raw data duration	All debug settings are disabled after this period.	1 min	720 mins	30 mins
Raw data log mode	• Last iteration - Detector ADC raw data will be logged by overwriting data of previous iteration. • All iterations - Detector ADC raw data will be logged into new folders for each scan iteration.	-	-	Last iteration
Spectral post-processing logs	Write pre and post processed data of spectral processing logic into file system	-	-	Disable
Log additional debug parameters advanced	Logs additional parameters into Reports under the Debug parameters section to facilitate troubleshooting			Disable
PM2 Key metrics monitoring advanced	Enable streaming of key metrics to https://app.pm2.io this requires the system to be connected to the internet.			Disable

Table 16. Debug parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Logging				
Print Debug logs	Setting to enable/disable debug logs			Disable
Debug timeout duration	The duration (Hours) after which debug logs will disable itself.	0.1 hours	72 hours	1 hour
Enable Multi-Level Logging	Print all logs if set true else depending on MACHINE_CONST_DEBUG_PRINTS debug logs may be omitted	-	-	Disable
Diagnostics				
Digital diagnostic at init	Enable/Disable digital diagnostic check during initialize.	-	-	Enable
Analog diagnostic at init	Enable/Disable analog diagnostic check during initialize.	-	-	Enable
Voltage test tolerance	Acceptable tolerance of measured voltage against requested voltage.	0 %	100 %	10 %
Calibration test step size	Step size for sweeping signal voltages to check calibration.	1 V	100 V	10 V

1.4.3.5 Detector

Table 17. Detector parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Background correction				
Log background scan data into reports	Enable/disable the writing of background scan data into the report file	-	-	Disable
Log background scan data into reports	Enable/disable the writing of background scan data into the report file	-	-	Disable

Background scan mass selection mode	Background scan mass selection mode for SIM/Molecule scan in non-range cases • 1- Scan selective masses • 2- Scan all foreground masses • 3 - Scan minimal foreground masses			Scan selective masses
Background masses to scan for non-range masses	Background masses to scan for non-range masses	-	-	10, 15, 20
Dwell time for background selective masses	Dwell time for background selective masses	2	2000	32

Table 17. Detector parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Background correction				
Minimum mass range in SIM mode to apply s-golay	Minimum masses in SIM scan to apply s-golay algorithm for background correction. In case of multiple ranges each range needs to suffice condition to apply s-golay.	30 s	3500 s	60 s
Spectral smoothing				
Spectral smoothing (moving average)	Smoothen the spectrum along the mass axis by calculating a moving average.	-	-	Disable
Moving average window size	Spectral smoothing moving average window size.	3	7	5

Noise filtering

Normalize ion current with emission	Ion current is normalized with emission current to account for minor fluctuations in emission. Emission current is sampled once every Hardware monitor and control interval.	-	-	Disable
Ion current noise filtration mode	Select the required method from the drop-down list. Methods are: • 1 - Basic method (linear) • 2 - Generic noise filter (difference) • 3 - Periodic average of differences	-	-	Basic method (linear)
Noise frequency	Used for filtering AC line/pump noise.	0 Hz	100 Hz	50 Hz

Relay controls

nMOS1 Off to pMOS1 On duration	Duration for which nMOS is switched Off for reset relay (RLY1_NMOS_CTRL_FROM _UC is held low for specified duration).	1 us	1000 us	30 us
pMOS1 On duration	Duration for which pMOS is held in On state for reset relay (RLY1_CTRL_FROM_UC held low for specified duration).	1 us	1000 us	300 us
pMOS1 Off to nMOS1 On duration	Duration for which pMOS is held in Off state before nMOS is switched On for reset relay (Time between RLY1_CTRL_FROM_UC set high to RLY1_NMOS_CTRL_FROM_UC set high).	0 us	30 us	22 us

Table 17. Detector parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
nMOS1 On duration	Duration for which nMOS is held in On state for reset relay (RLY1_NMOS_CTRL_FROM_UC is held high for specified duration).	0 µs	1000 µs	50 µs
nMOS2 Off to pMOS2 On duration	Duration for which nMOS is switched Off for range relay (RLY2_NMOS_CTRL_FROM_UC is held low for specified duration).	1 µs	1000 µs	30 µs
pMOS2 On duration	Duration for which pMOS is held in On state for range relay (RLY2_CTRL_FROM_UC held low for specified duration).	1 us	1000 µs	300 µs
pMOS2 Off to nMOS2 On duration	Duration for which pMOS is held in Off state before nMOS is switched On for range relay (Time between RLY2_CTRL_FROM_UC set high to RLY2_NMOS_CTRL_FROM_UC set high).	0 µs	30 µs	22 µs
nMOS2 On duration	Duration for which nMOS is held in On state for range relay (RLY2_NMOS_CTRL_FROM_UC is held high for specified duration).	0 µs	1000 µs	50 µs
Capacitor				
Capacitor switching	Enable dynamic capacitance switching between 1 pF and 100 pF capacitor to improve ion current estimation accuracy.	-	-	Disable
Consecutive capacitor reset count	Number of consecutive resets issued by the micro-controller for a single reset request from the SoC.	1 s	5 s	1 s
Calibrated value of 10 pF Capacitor	The capacitance value is ideally 10 pF. Deviations are calibrated and corrected in this field.	0.1 pF	200 pF	10 pF
1 pF capacitor max reset attempts	Maximum number of resets permitted per estimation of ion current for 1 pF capacitor. The number of ramps is one greater than this value.	0 s	1000 s	10 s
100 pF capacitor max reset attempts	Maximum number of resets permitted per estimation of ion current for 100 pF capacitor. The number of ramps is one greater than this value.	0 s	1000 s	5 s
1 pF saturation detection samples count	Number of samples that should cross the capacitor reset voltage before a reset is issued for the 1 pF capacitor.	1 s	100 s	1 s

	This prevents false alerts for saturation.			
100 pF saturation detection samples count	Number of samples that should cross the capacitor reset voltage before a reset is issued for the 100 pF capacitor This prevents false alerts for saturation.	1 s	100 s	5 s

Table 17. Detector parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Averaging				
Ion Current averaging	Enable or disable averaging of ion current data of a mass with multiple samples to eliminate high frequency noise components	-	-	Disable
Ion current averaging window size	Number of samples of ion current of specific mass used to compute the average.	2	100	3
Others				
Voltage ramp bottom ignore	ADC samples to ignore from the bottom of the ramp used to estimate ion current.	0 %	100 %	0 %
Voltage ramp top ignore	ADC samples to ignore from the top of the ramp used to estimate ion current.	0 %	100 %	0 %

1.4.3.6 System

Table 18. System parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Controller fan				
Fan Control Mode	• 0 - PWM duty cycle control. • 1 - Speed control. • 2 - Temperature control.	-	-	PWM duty cycle control
Fan Duty Cycle Set Point	PWM Duty cycle at which the fan is run. Active only when Fan control mode is set to Duty cycle control.	30	100	100

Measurement Units				
Pressure unit	SI and non-SI units of pressure.	-	-	Pa
Temperature unit	SI and non-SI units of temperature.	-	-	Kelvin
Time				
System date format	Formatting for display and recording of date and time in the system.	-	-	YYYY-MM-DD
System time format	Formatting for display and recording of time in the system.			HH:mm:ss
Set Internet time	Fetch time from a time server.	-	-	Enable
System date & time	Set system time.			
Network				
Hostname	Show/edit hostname of the system.	-	-	amsdev-9999.atoms.app

Table 18. System parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
SSH access	SSH is used to remotely connect to the system to debug issues. By default, SSH access is disabled. It can be enabled by selecting the appropriate option from the drop-down menu and setting it.	-	-	Disable SSH (persistent)
Ethernet IP address	Show/edit IP address of the system.	-	-	show current IP
Ethernet MAC address	Show/edit MAC address of the system.	-	-	show current MAC
Ethernet IP configuration mode	Configures the IP assignment mode.	-	-	DHCP Server

General				
System name	Show/edit system name of the system.			amsdev-9999.atoms.app
UI				
Disable GUI actions in CLI/Modbus modes	Disable user interaction with the UI when AMS is communicating through CLI or Modbus interface.	-	-	Disable
Auto-restart scan after power failure resume	Auto restarts scan during AMS-manager, SoC/uC restart or power failure.	-	-	Disable
Control panel polling period	Periodicity of polling fields in the control panel.	1 s	3600 s	1 s
Maximum data points in trend plot	Maximum data points in a plot.	1000	250000	10000
Down sampling algorithm	Methods supported are- ASAP- Automatic Smoothing for Attention Prioritization SMA- Simple moving average LTTB- Largest triangle three buckets LTOB- Largest triangle one bucket LTD- Largest triangle dynamic			LTTB
Session auto-override timeout	Time to wait for the active user's reply before auto-overriding.	10 s	120 s	30 s

Table 18. System parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Characterization				
System Characterization	System characterization features-\n Negative ion current estimation	-	-	Enable
Reference mass for raw data analysis	Mass to be considered for raw data analysis.	0 amu	250 amu	10 amu

Idle state settings (Note: The password protected fields are only for Atonarp engineers to use)

Filament current	Filament current to be set when the system is in idle state.	0 A	4 A	1 A
Quad RF voltage	RF voltage to be set when the system is in idle state.	0 V	500 V	117.46 V
Quad RF frequency	RF frequency to be set when the system is in idle state.	0 MHz	20 MHz	3.5 MHz
Filament bias voltage	Filament bias voltage to be set when the system is in idle state.	0 V	160 V	10 V
Box bias voltage	Box bias voltage to be set when the system is in idle state.	0 V	160 V	150 V
Lens bias voltage	Lens bias voltage to be set when the system is in idle state.	0 V	160 V	143 V
DC Differential Voltage	DC diff voltage to be set when the system is in idle state.	0 V	160 V	19.57 V
DC Plus Fine Correction Voltage	DC plus fine voltage to be set when system is in idle state	-5 v	7 v	0 v
DC Minus Fine Correction Voltage	DC minus fine voltage to be set when system is in idle state	-5 v	7 v	0 v

Data Retention

Scan Data Retention	Scan data will be preserved on the system for given number of days	14 days	35 days	21 days
Monitored Data Retention	Monitored data will be preserved on the system for given number of days	7 days	35 days	14 days
Debug Data Retention	Debug data will be preserved on the system for given number of days	1 day	7 days	1 day

SKU

Ion Detector Mode	Select the required method from the drop-down list. Methods are:\n• 0 - Faraday Cup\n• 1 – SEM			SEM

Table 18. System parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
SKU				
SEM Auto Range	Ion detector SEM auto range selection			FALSE
Ion detector TIA range selection	Ion detector TIA range selection			Range 1
TIA SEM Slope Range 1	TIA SEM Slope Range 1	-1000	1000	-2.00E-09
TIA SEM Intercept Range 1	TIA SEM Intercept Range 1	-1000	1000	0
TIA SEM Gain Range 1	TIA SEM Gain Range 1	-1000	1000	1
Ignore initial samples in TIA	Number of initial samples needs to be ignored in case of TIA mode	0	500	0

1.4.3.7 Drive Board

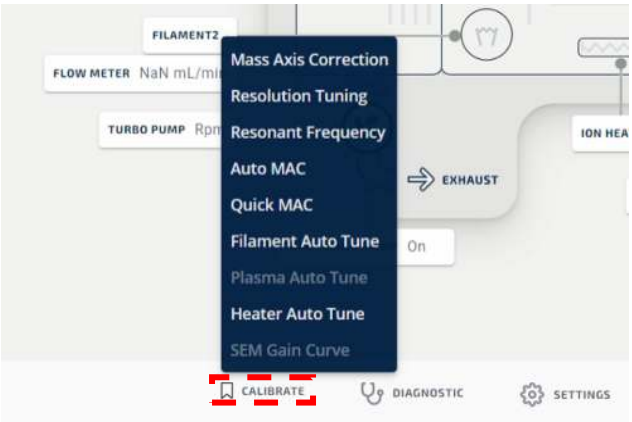
Table 19. Drive board parameter description

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Electric Lens				
EL1 Voltage	Set EL1 lens Voltage	-180	0	-90
EL2 Voltage	Set EL2 lens Voltage	0	180	50
Safety				
Safety Pressure Theshold-1	Pressure threshold to safeguard sem and Ion source	0	2000	1.00E-02
Safety Pressure Theshold-2	Pressure extended threshold to safeguard sem and Ion source	0	2000	5.00E-02
Safety Pressure Theshold-3	Pressure threshold to safeguard Heaters	0	2000	1.00E+00
Safety Pressure Theshold-4	Pressure threshold to safeguard Turbo Pump	0	2000	1.33E+03

1.4.4 Calibration

As an analytical instrument producing signal abundance (Y-axis) as each atomic mass unit (X-axis), Aston requires calibration to obtain the most accurate quantitation (partial pressures) for specific compounds. The calibration is usually performed using a gas mixture. The selection of the appropriate mixture of components depends on the mass range over which the calibration is desired.

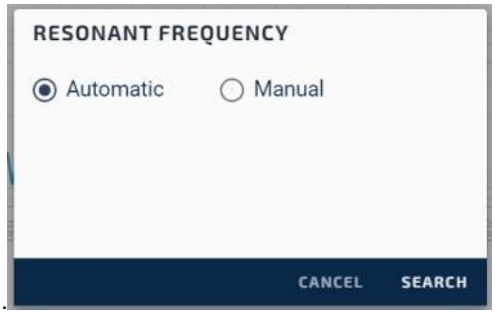
Here, spectral calibration procedures are the main topic of focus, accessible at the bottom of the dashboard. Aston units are factory calibrated and calibration (for Mass-axis and Resolution tuning) files(in csv format)are locally stored and can be readily accessed.

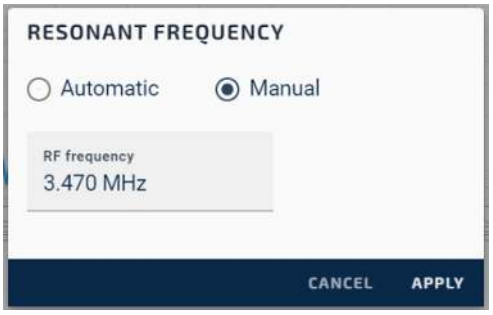


Aston spectral calibration focuses on 3 steps: Resonant frequency search, Resolution & sensitivity tuning, Mass axis correction

1.4.4.1 Resonant frequency

As mentioned above the resonant frequency calibration is performed at the factory and this procedure should be considered a verification only step. The Resonant Frequency can be set through Automatic or Manual options. Using the Automatic option, the system determines the resonant frequency through a few seconds long computer controller tuning procedure. The resonant frequency is then displayed and is usually in the 3.4-3.6 MHz range. The user can then apply or discard the value.



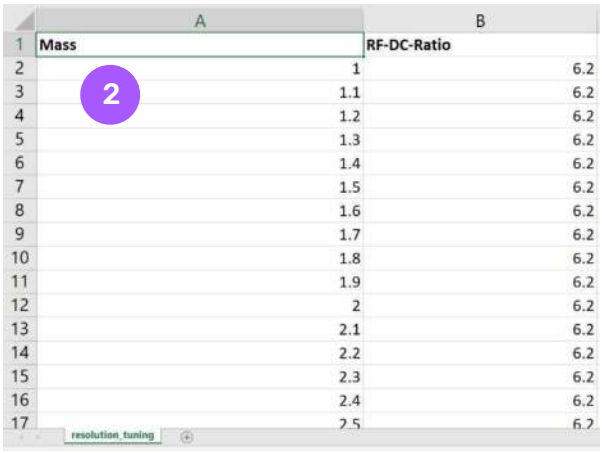


Under Manual, the user can input a custom RF frequency value. The Manual option of setting the frequency should only be used by advanced users as far off values can cause overheating of the RF circuitry.

1.4.4.2 Resolution Tuning

The RESOLUTION TUNING function enables the user to set a RF-DC ratio schedule to achieve a target peak width for the entire mass range. RF/DC values can be set using Enable tune from file. The tuning is accomplished using the following steps:

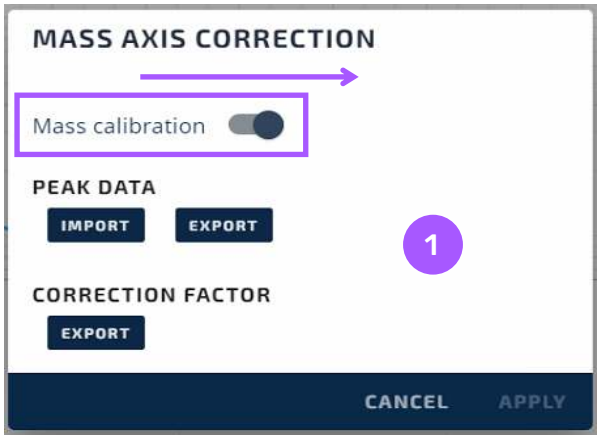
1. Below TUNE, click on **EXPORT** and make note of the path that appears on the bottom left of the screen. The exported template will be saved in the local Aston folder.
2. The exported resolution tuning template (shown below) has Mass and RF-DC ratio fields wherein the user can modify the RF-DC ratio values
3. After setting RF-DC ratio values for the entire mass range, click on **IMPORT** to upload the XLSX file
4. Use the High Resolution/High Sensitivity slider to set the target peak width
5. Click on **PROCEED**



	A	B
1	Mass	RF-DC-Ratio
2	1	6.2
3	1.1	6.2
4	1.2	6.2
5	1.3	6.2
6	1.4	6.2
7	1.5	6.2
8	1.6	6.2
9	1.7	6.2
10	1.8	6.2
11	1.9	6.2
12	2	6.2
13	2.1	6.2
14	2.2	6.2
15	2.3	6.2
16	2.4	6.2
17	2.5	6.2

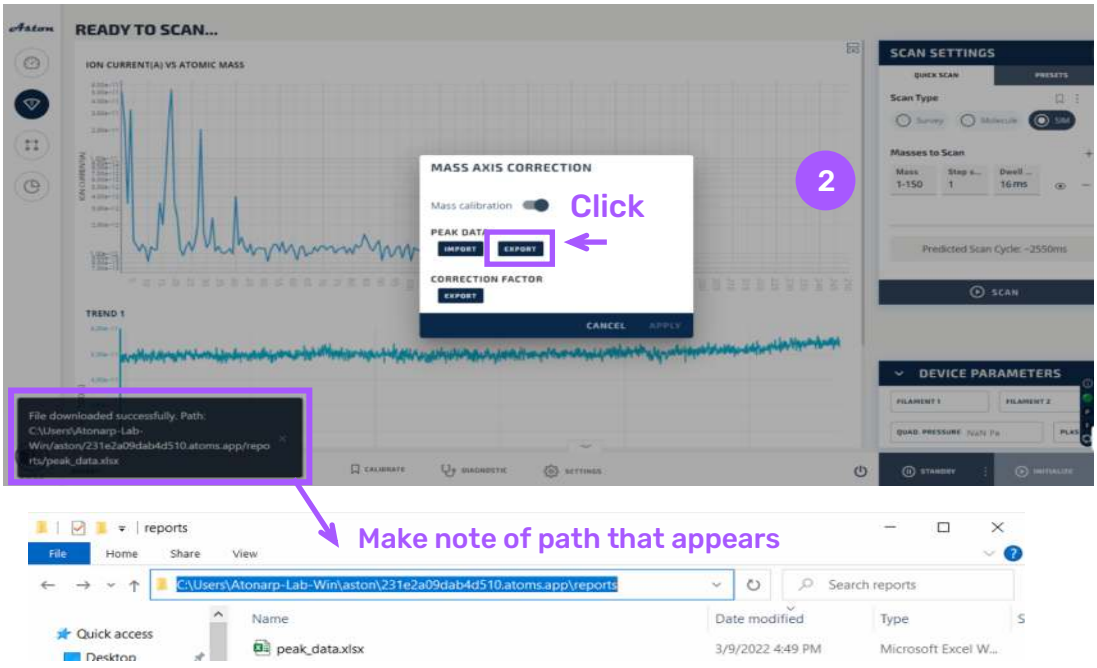
1.4.4.3 Mass axis correction

The MASS AXIS CORRECTION function enables the user to correct for peak location errors across the mass spectrum. Enabling Mass calibration lets the user import and export calibration files. The user can make changes to the spreadsheet under Excel in the exported .csv file and import it to apply new calibration. The correction is accomplished using the following steps:

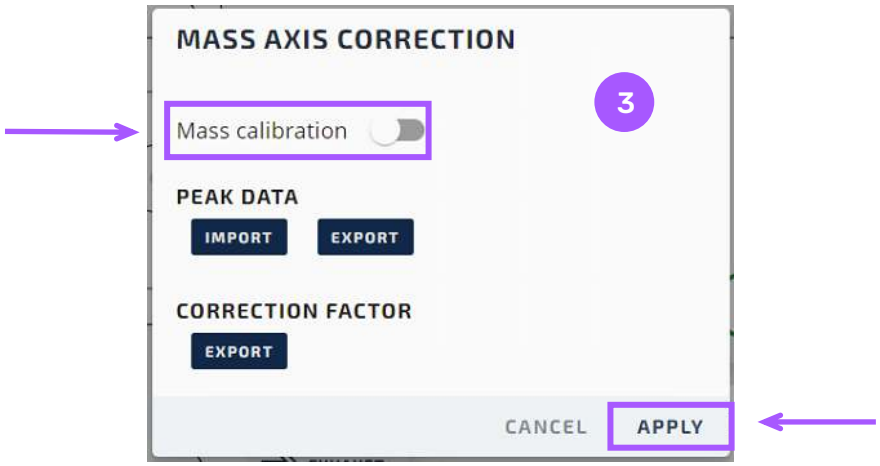


1. Ensure Mass calibration is enabled. Enable/disable Mass calibration by toggling this field. The settings from the imported file are applied when enabled.

2. Click on **EXPORT** and make note of the path that appears on the bottom left of the screen. This is the location where the peak_data.xlsx file will be downloaded.

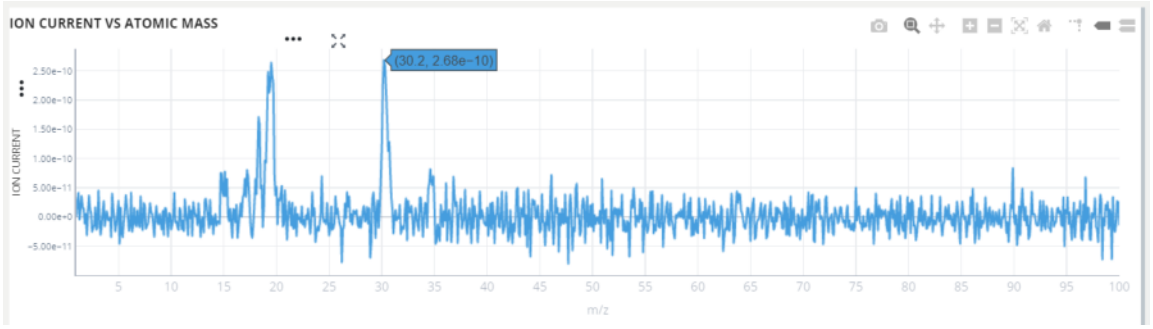


Disable mass calibration and click on APPLY.



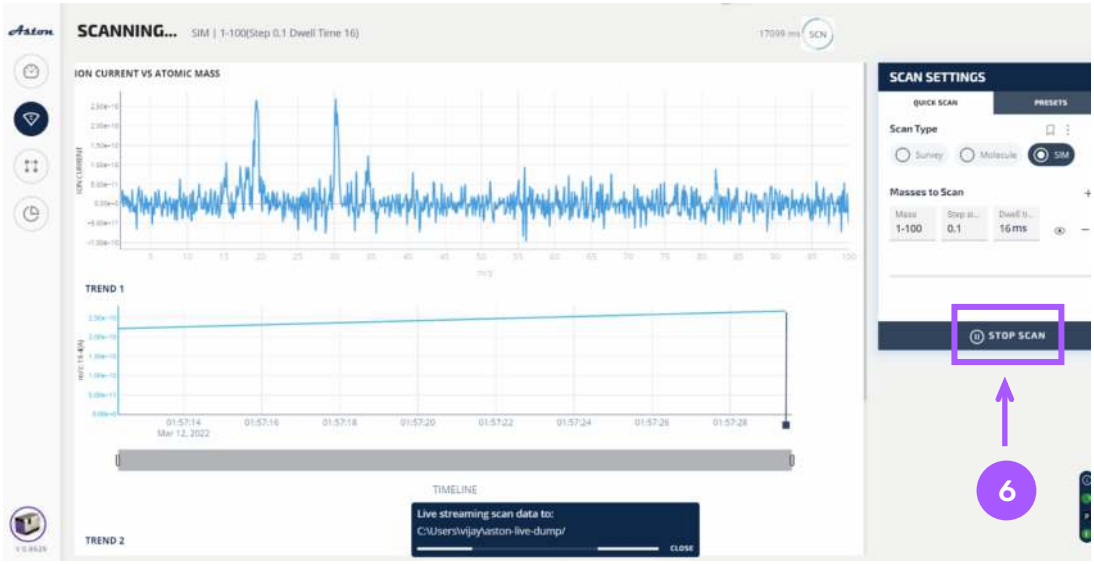
3. Navigate to the SCAN tab and click on SCAN.

4. Look at scan data and identify a peak of interest. As an example, the figure below shows a peak at 30.2 m/z. This peak corresponds to Nitrogen and thus should be at 28 m/z instead.
5. Now turn to the peak_data.xlsx file. In it there will be two columns: Reference mass and



User-observed mass. Continuing with the previous example, the user will input the observed mass (30.2) next to the reference mass (28), as shown below. Save the file. Repeat the steps for all reference masses/peaks being calibrated for.

6. Once all masses have been appropriately located and corrected for, stop the current scan, and open the Mass Axis Correction function again.



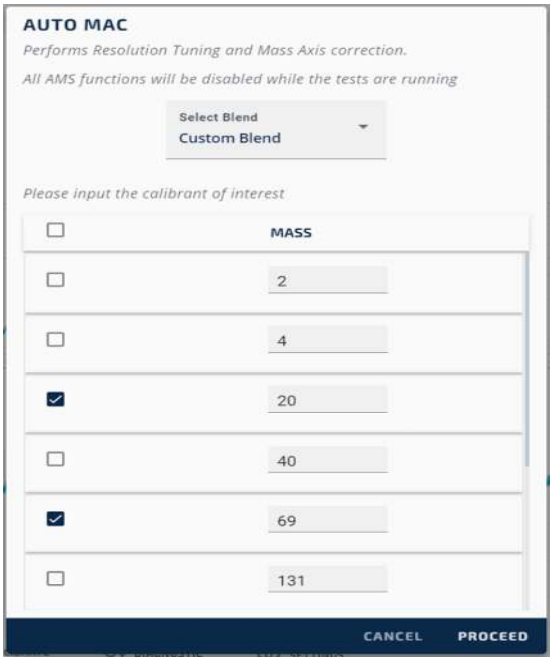
7. Enable Mass calibration, click on IMPORT to upload the newly saved peak_data.xlsx, and then click APPLY. The embedded algorithm in AtonLabAstonApp software will now perform the necessary corrections.
8. The CORRECTION FACTOR can be exported by clicking on the EXPORT button. The Exported XLSX file will be saved in the local folder.

Exported correction factor

A	B
Mass	**RF correction**
1	1
1.1	1
1.2	1
1.3	1
1.4	1
1.5	1
1.6	1
1.7	1
1.8	1
1.9	1
2	1
2.1	1
2.2	1
2.3	1
2.4	1
2.5	1

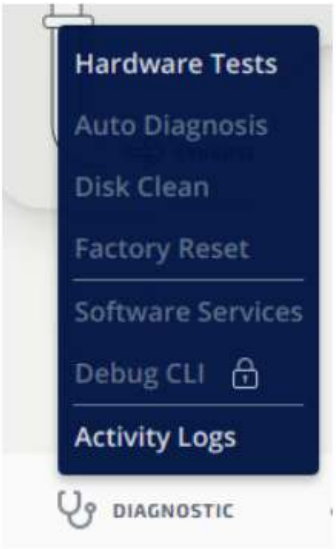
1.4.4.4 Auto MAC

The Auto MAC function is a computer automated method for calibrating an Aston system. Auto MAC steps through Resonant Frequency, Resolution Tuning, and Mass Axis Correction procedures internally via an advanced algorithm. Under Auto MAC, the system performs the three steps using a single source of gas mixture. It allows the user to select from some preloaded gasses e.g., Argon and PFTBA or a custom gas blend that can be defined. Once the calibration gas is selected, click on the PROCEED button.



1.4.5 Diagnostic

The Diagnostic menu allows the user to perform a basic diagnostic check on the Aston Impact software. Some of the options are disabled and would be made available in later software releases.



1.4.5.1 Hardware Tests

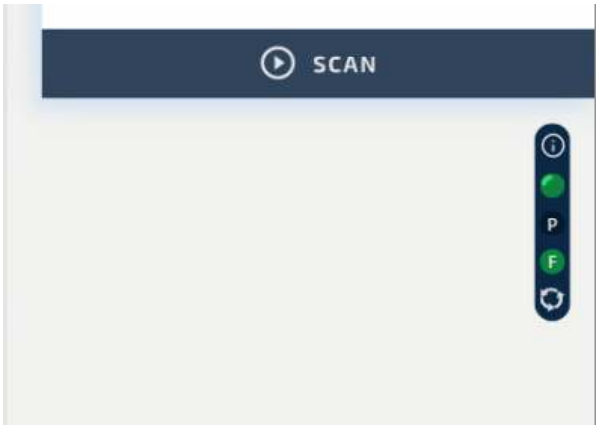
The hardware tests options execute a series of hardware diagnostic tests that include voltage and eeprom checks. The report can be downloaded from the Reports section. Please refer Section 7.9.3

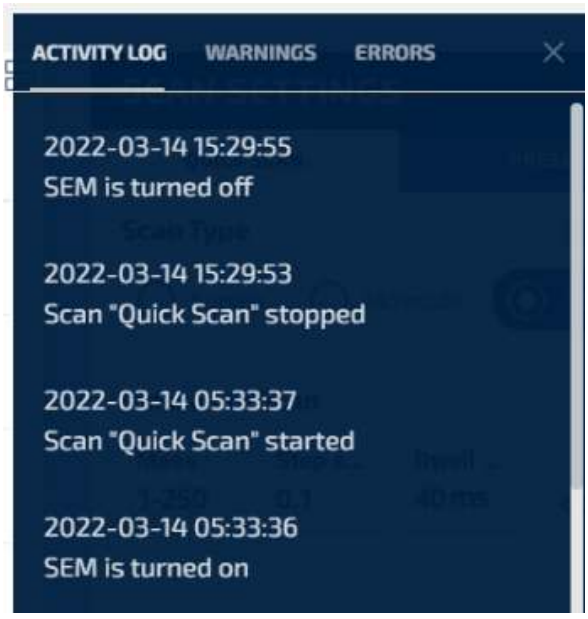
1.4.5.2 Activity Logs

The Activity Logs allows the user to view the real time events, warnings, and errors in the Aston Impact system as they happen.

All events in the system are logged to the activity panel with timestamp and appropriate messages.

For any new notifications > error, warning, activity logs indication is logged to the micro panel. Error tab has the error messages and recommended action to proceed
This a floating panel docked at right bottom of the screen.





1.4.6 Initialize

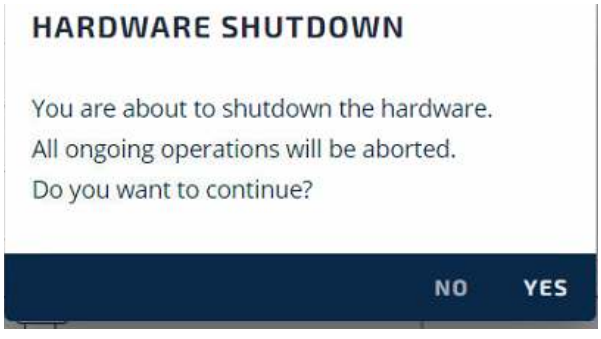
Initialize workflow allows the user to put the Aston Impact unit on a Scan Ready state. The Default initialize workflow sets filament 1 set point to 400µA. The Aston Impact unit is expected to be in Scan Ready to execute a scan.

1.4.7 Stand By

Standby Workflow allows the user to put the Aston Impact unit to a System Ready state. While in the System Ready state, scans cannot be executed.

1.4.8. Hardware shutdown and reboot interface

Users now have the option to shut down hardware and reboot the interface from the dashboard itself. When a user clicks on the shutdown option a message lthe ike below prompts before shutdown. All the operations will be aborted. User needs to save data and then shut down the hardware.



1.4.9. Error Handling

The error notifications help the users to identify the errors that occur during the process.

1.5. System

The System menu allows the user to view the Aston Impact system details

1.5.1 System Update

Users can access the system update through

Main Menu >> Aston Impact Button >> System Update.
The System Update section allows the user to update board calibration binary from the UI. Users have the option to choose different board calibration i.e., Front panel, Ion detector, Power supply, Ion drive and RF drive. Users can export board calibration files.

Exported Ion Drive template

	A	B	C
1	Signal	Slope	Intercept
2	DCDIFF_DAC	41	0
3	DCMINUS_ADC	54.10409164	2.053296566
4	EMISSION_CURRENT_ADC(LS)	8200	0
5	EMISSION_CURRENT_ADC(HS)	8100	0
6	FILAMENT1_VOLTAGE_ADC	0.931200027	0.0056
7	FILAMENT2_VOLTAGE_ADC	1.091400027	-0.0064
8	DCPLUS_FINE_CORRECTION_DA	-4.489999771	13.75199986
9	DCMINUS_FINE_CORRECTION_I	-4.489999771	13.75199986
10	FILAMENT_CURRENT_ADC	4.325799942	0.047499999
11	DCDIFF_ADC	84.71900177	-0.0042
12	DCMINUS_FINE_CORRECTION_A	30.87999916	0.199000001
13	DCPLUS_FINE_CORRECTION_AD	30.87000084	0.200000003
14	LENSBIAS_DAC	25.98543167	0.020382229
15	LENSBIAS_ADC	54.20362473	0.005804631
16	BOXBIAS_DAC	25.28503036	-0.035323974
17	BOXBIAS_ADC	53.96319962	-0.00750715
18	FILBIAS_DAC	-49.94630432	104.4301987
19	FILBIAS_ADC	54.33312225	2.724486589
20	DCPLUS_ADC	126.7118988	0.01407907
21	DCPLUS_DAC	51	0.019234616
22	DCMINUS_DAC	-49.98168182	104.3620987

User has option to change/update the system time zone

Offline upgrade

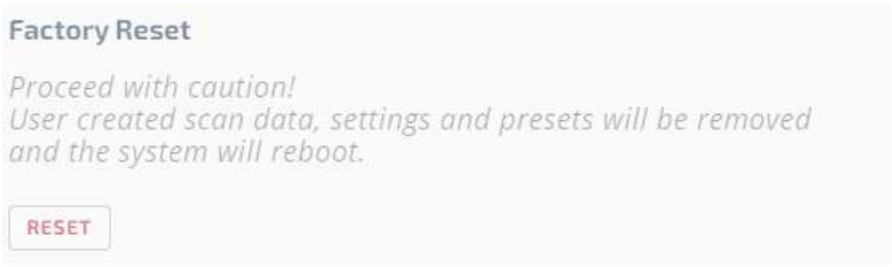
Users can update firmware through the firmware update option where users can see the current version of the Aston Impact and can check for the update. Users can update the system offline by clicking on choose file button and the user needs to choose (.atp) file and update the system.

Main Menu Aston Impact Button >> System Update >> Firmware Update >> Choose File (.atp)

Factory reset

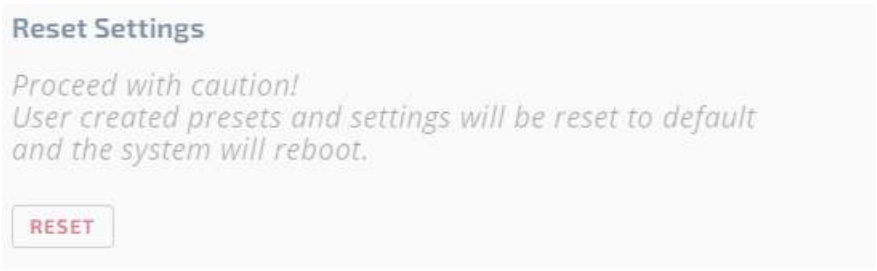
Users have provision to factory reset the system. This should be done with caution as all the user created data, settings and presets will be removed permanently and the system will reboot. User has to choose it only if required.

Main Menu Aston Impact Button >> System Update >> Factory reset >> Reset



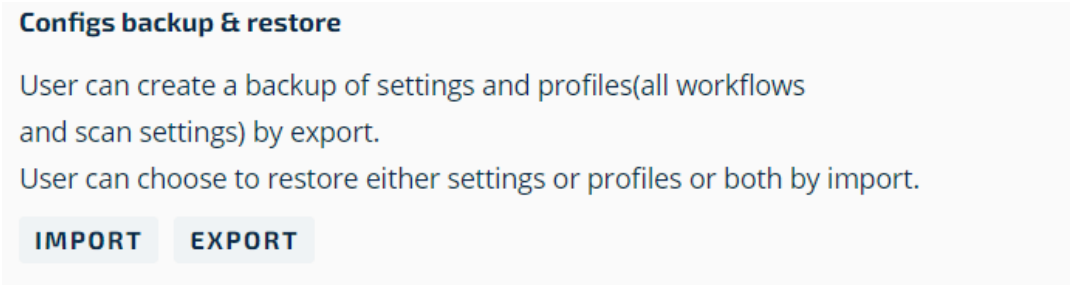
Like factory reset, the reset settings option will reset all the user defined presets and settings to default. The system will reboot upon reset. This should be done with caution as all the settings will be removed from the system.

Main Menu Aston Impact Button >> System Update >> Reset settings >> Reset



Users can configure backup and restore the settings. Users have the option to export settings and profiles i.e., workflows and scan settings. Users can restore the settings and profiles or both by import option. Exported settings or profiles will be saved in the Aston Impact local folder.

Main Menu Aston Impact Button >> System Update >> Configs backup and restore >> Choose import or export.



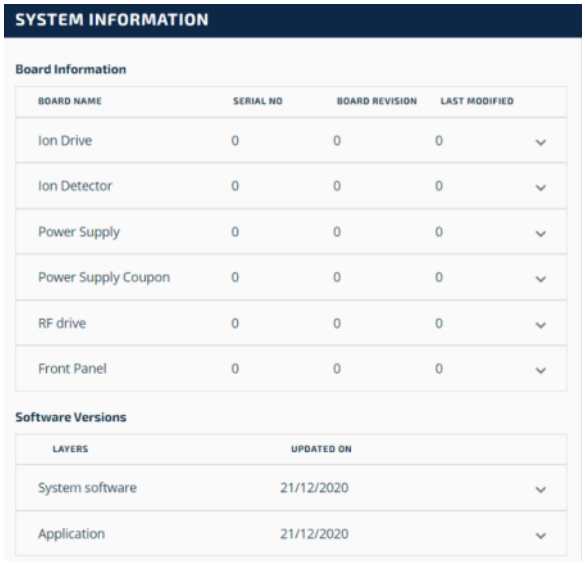
Things to consider before Online/Offline Upgrades

1. All data will be removed from the system (user defined settings, presets, profiles, etc.)
2. While downloading certain files like .exe. users may get warning messages. User needs to mention it as safe and download the package.

3. After updating the firmware users should load fresh app to access Aston Impact UI.
4. For integrated methods like Modbus & gRPC updated documents, sample clients are provided. For gRPC, updated stub files need to be integrated.

1.5.2 System Information

The system information sections describe the Aston Impact Software and PCB board revisions. Each row can be expanded to view detailed descriptions.



1.6 Plots

Plot charts are present in multiple pages of the user interface. The feature design of plots is mostly consistent across the pages. Charts have a hierarchical arrangement of properties: Panel properties > Chart properties > Axis properties

1.6.1 Plot Type

- Spectral chart: A plot of ion currents measured against the m/z's scanned.
- Trends chart: A plot of signals varying as a function of time.

1.6.2 Plot properties

1.6.2.1 Spectral plot

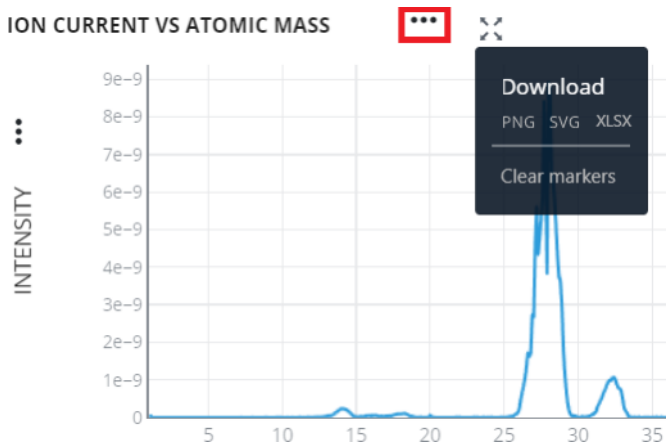
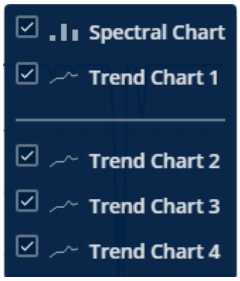


Table 25. Spectral plot settings

PARAMETER	DESCRIPTION
Download plot as PNG, SVG, XLSX	Download the plot of the currently running scan in the selected format.

1.6.2.2 Trends plot

Trend signals



Markers

Table 26. Trends plot settings

PARAMETER	DESCRIPTION
Trends	User can enable/disable up to four y-axes - Left 1, Left 2, Right 1, Right 2 De-selecting a Y axis will unload any data cached into memory corresponding to the axis. It is recommended to hide instead of unload to reduce time penalty incurred with reloading large datasets. An axis can be hidden by clicking on its legend. NOTE: Up to a maximum of 4 trend signals can be visualized in a page. The 4 signals can be within a single trend chart or one each across 4 trend charts. Each chart can show up to 250,000 samples (default, can be adjusted from Aston settings) per signal. The system will sub-sample the data. This is done for performance reasons.
Download plot as PNG, SVG, XLSX	Download the plot of the currently running scan.

1.6.3 Axis properties

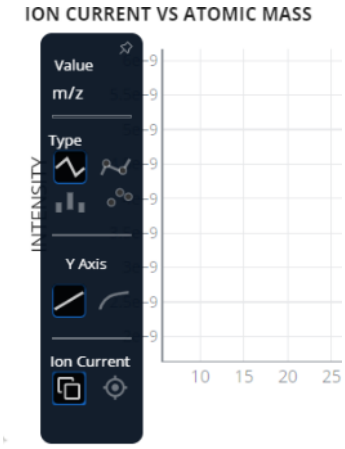


Table 27. Plot settings

PARAMETER	DESCRIPTION
Signal	The user can select a signal to associate with the specific Y axis. The signal may be ion currents of a specific mass or other system properties like pressure, temperature etc. This field is not applicable for spectral charts.
Type	Select between lines connecting samples, points showing samples, lines and points, or a bar chart.
Y-Axis: Linear Scale	Each axis marker is equidistant from the adjacent markers and increases by a fixed unit of measurement. The unit is auto scaled to best visualize the signal.
Y-Axis: Logarithmic scale	The primary axis markers have values separated by a factor of 10. Intermediary markers may not be equidistant from the neighbors. This scale is useful to visualize a large dynamic range of signals within a single plot.
Ion current: Relative value	Ion currents are displayed with the highest peak signal at 100% and all else relative to this signal.
Ion current: Absolute value	Ion currents as measured from the detection circuit in units of Amperes.
Edit label	The user can edit the Y axis label for ease of reference.

NOTE

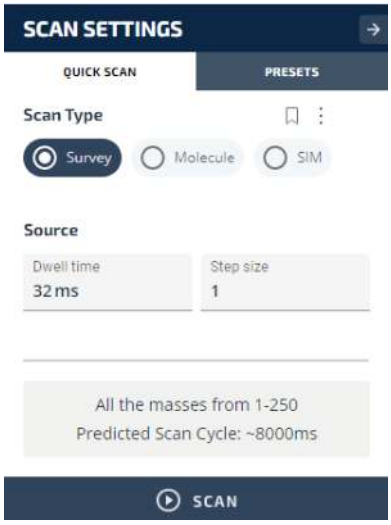
System sub-sample data to show only a limited number of samples in the chart. This number can be adjusted by setting the parameter "Maximum data points in trend plot".

1.7 Scan

In order for the user to run a scan, the Aston Impact system has to be in Scan Ready state. Please refer to the xxx section to put the system to scan ready state.

1.7.1 Scan Settings

The Scan Settings panel allows the user to bring together frequently used mass spectrometer settings like dwell times, masses/molecules of interest, modes of scan etc. and test them and save them as presets for reuse for various application needs.



1.7.1.1 Quick Scan

This feature is used to make settings changes and immediately test them without saving them as a preset.

Survey scan type

Survey Scan - For range scans with user customizable dwell time and step size input. Range needs to be updated in AMS Settings >> Mass Filter >> Max Mass range.

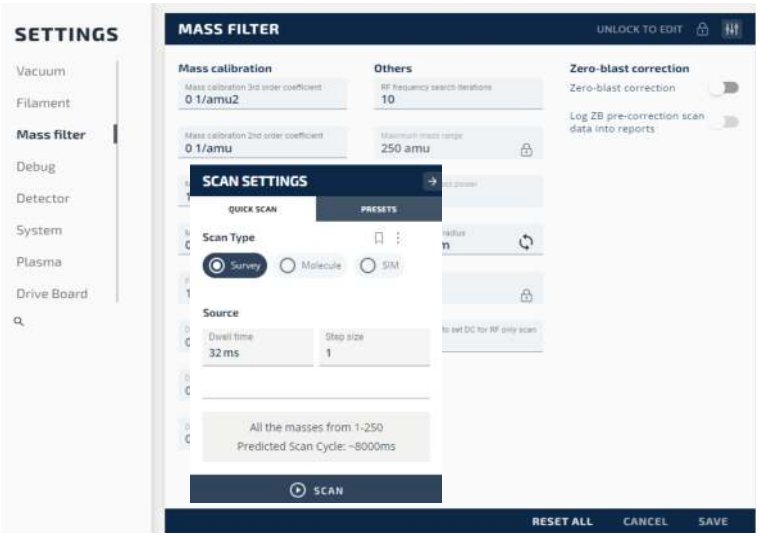


Table 28. Survey scan type

PARAMETER	DESCRIPTION
Scan type	Survey: Scan all masses of all analytes for which model (B/PTCR) data is available. This mode typically scans 1-250 amu (unless a B/PTCR model is generated with fewer masses).
Source	Ion source: • Filament1 • Filament2
Dwell time	The maximum time spent at each mass obtaining samples for ion current estimation. Minimum time is 10 ms and maximum 2000 ms. Default is 32 ms. Note: The total scan time for a mass is the sum of dwell time and scan overheads associated with processing and transmission of the data. Typical scan overheads range from 4 -10 ms.
Step	Defines scan resolution as low as 0.1 mass. Note: 1) This option is available when the scan type is Survey and SIM. 2) 0.1 step size is the same as 10 ppamu. 1 step size is the same as 1 ppamu. 0.3 step size is the same step size as 3 ppamu, but the masses scanned are different. Example, If the user specifies a SIM range of 1-2 with a step size of 0.3, it will scan 1, 1.3, 1.6, 1.9 amu. If the user specifies these independent mass values for SIM like 2, 3, 4, then scan masses 1.7, 2, 2.3, 2.7, 3, 3.3, 3.7, 4, 4.3.
Scan	Start or stop scan.

Molecule scan type

For Molecule specific scan with user customizable dwell time and No of Masses to Scan.

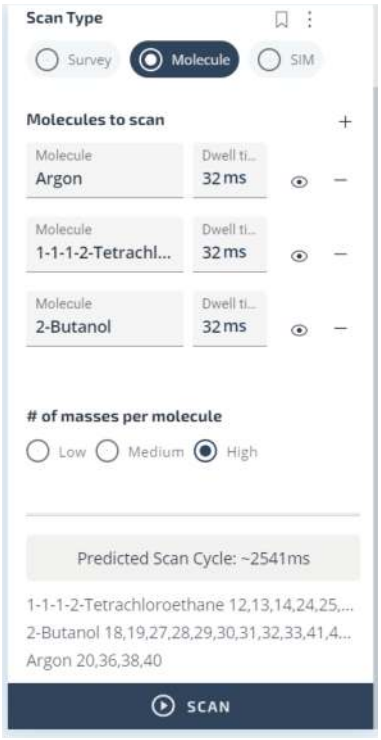


Table 29. Molecule scan type

PARAMETER	DESCRIPTION
Scan type	• Molecules: System automatically determines the least masses of interest for the molecules chosen. Mass selection accounts for convolution of signals from different analytes components at the same mass and automatically picks fragment peaks.
Source	Ion source: • Filament1 • Filament2
Dwell time	The maximum time spent at each mass obtaining samples for ion current estimation. Minimum time is 10 ms and maximum 2000 ms. Default is 32 ms. Note: The total scan time for a mass is the sum of dwell time and scan overheads associated with processing and transmission of the data. Typical scan overheads range from 4 -10 ms.
Molecules to scan	Select a sub-set of molecules to scan.
# of masses per molecule	• Low • Medium • High
Scan	Start or stop scan

SIM scan type

For options with range and single mass scans with user customizable dwell time and step size input.

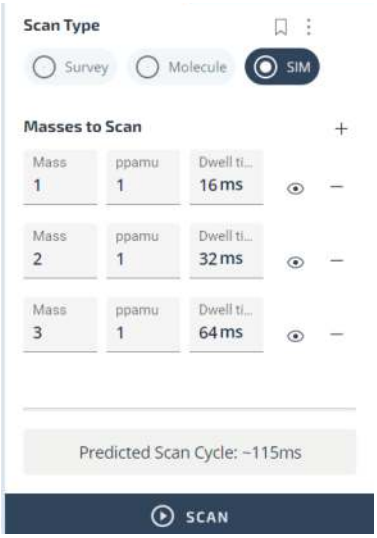


Table 30. SIM scan type

PARAMETER	DESCRIPTION
Scan type	SIM: Scans only user specified masses. No mole fraction is computed in this mode.
Source	Ion source: • Filament1 • Filament2
Dwell time	The maximum time spent at each mass obtaining samples for ion current estimation. Minimum time is 10 ms and maximum 2000 ms. Default is 32 ms. Note: The total scan time for a mass is the sum of dwell time and scan overheads associated with processing and transmission of the data. Typical scan overheads range from 4 -10 ms.
Masses to scan	Masses selected for scan. It cannot be empty and allows specifying one or more ranges of masses to scan or independent masses. Example: 8; 14-18;28. Note: This option is available when the scan type is SIM.
Scan	Start or stop scan.

1. *Click on the ellipsis button for more settings.*

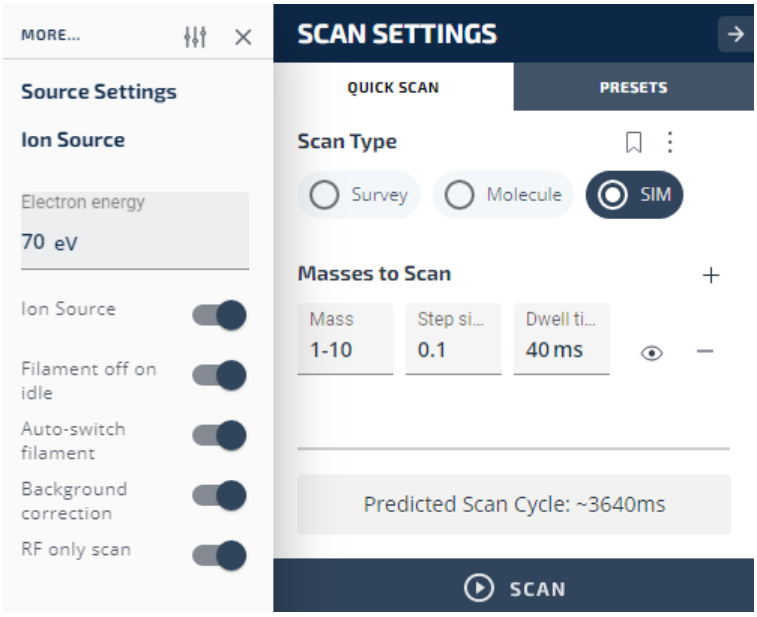


Table 31. More settings

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Source settings				
Electron energy	Energy imparted to electrons used for ionizing analyte molecules	35eV	80eV	70eV
Ion source	Turn the ion source, ON or OFF	-	-	Disable
FIlament off/on idle	Automatically switch off filament if idle	-	-	Disable
Auto switch filament	Automatically switch to another filament if one is broken	-	-	Enable
Noise				
Background correction	Enable or disable the background scan correction	-	-	Disable
RF only scan		-	-	Disable

2. *Click on the settings button for more setting parameter*

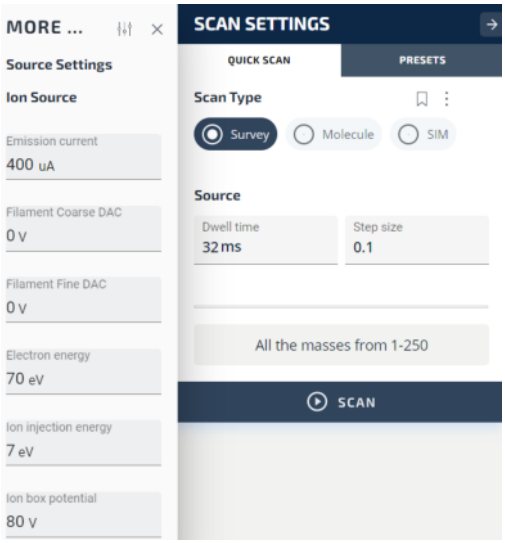


Table 32. More Advanced settings

PARAMETER	DESCRIPTION	MINIMUM	MAXIMUM	DEFAULT
Source settings				
Emission current	Current value of emission produced by the filament.	0.0 µA	10000 µA	400 µA
Filament coarse DAC	-	-	-	0 v
Filament fine DAC	-	-	-	0 v
Electron energy	Energy imparted to electrons used for ionizing analyte molecules.	35 eV	80 eV	70 eV
Ion injection energy	Energy imparted to the generated ions.	0 eV	15 eV	7 eV
Ion box potential	Potential of the box inside which ionization takes place.	120 V	160 V	80 V
Ion source	Turn the Ion source ON or OFF.	-	-	Disable
Filament off on idle	Automatically switch off filament if idle	-	-	Disable
Auto-switch filament	Automatically switch to another filament if one is broken	-	-	Disable
Background correction	Enable or disable the background scan correction.	-	-	Disable
RF only scan	A special scan mode that allows all ions to reach the detector without filtering to be used for diagnostics.			

1.7.2 Presets

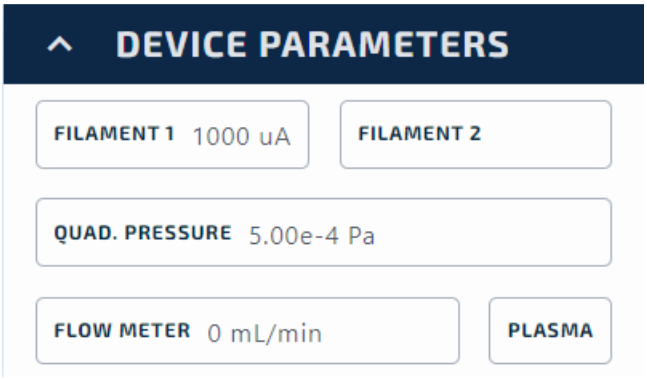
User can create a preset out of scan settings for reuse. Presets can be run independently or sequenced in workflows.

1.7.3 Plots

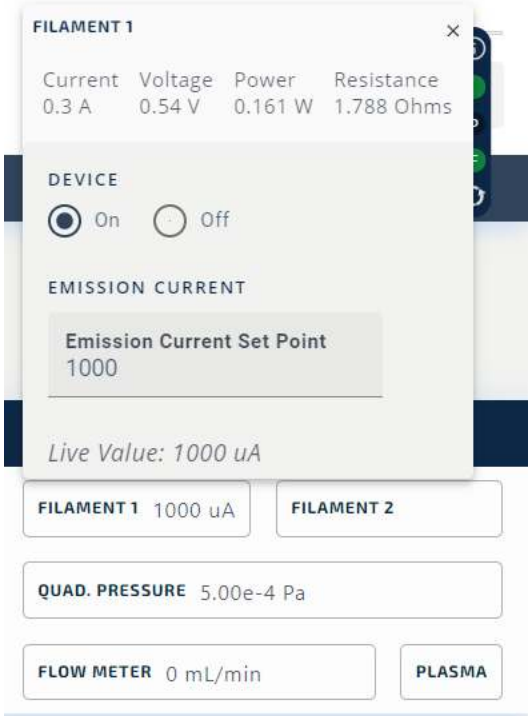
For more information about the plot settings refer to plots (section 7.6).

1.7.4 Device Parameters

Device parameters is the new option included in the scan page. Users can change the parameters without switching to the dashboard.



If a user wants to change the filament 1 parameters, then just a click on it opens up the filament 1 settings and the user can change it here (as shown in figure below). In the similar way users can change the device parameters for other options.

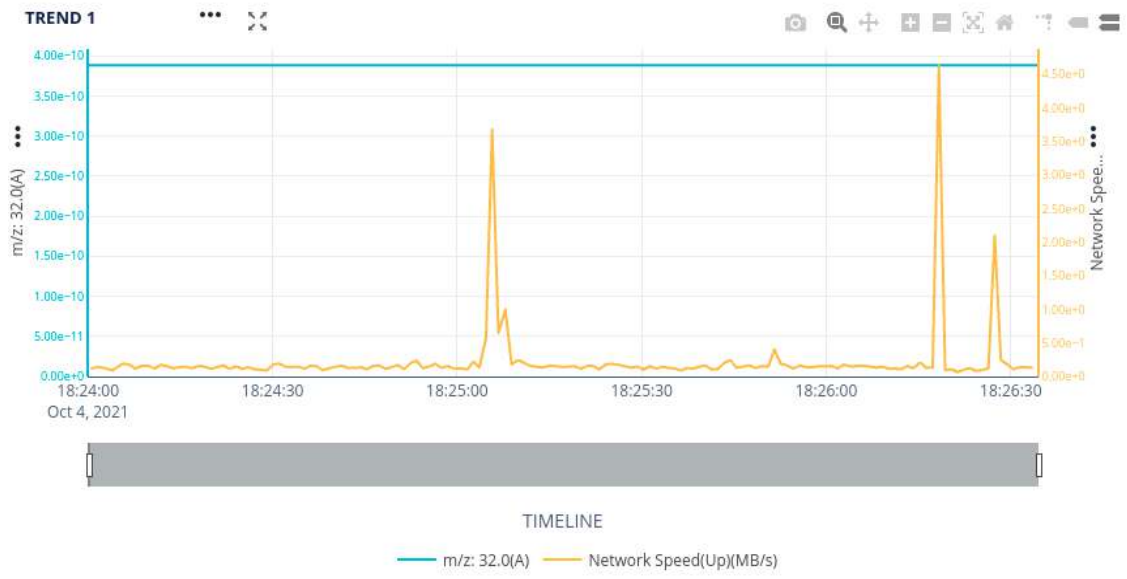


1.7.5 Residual Correction

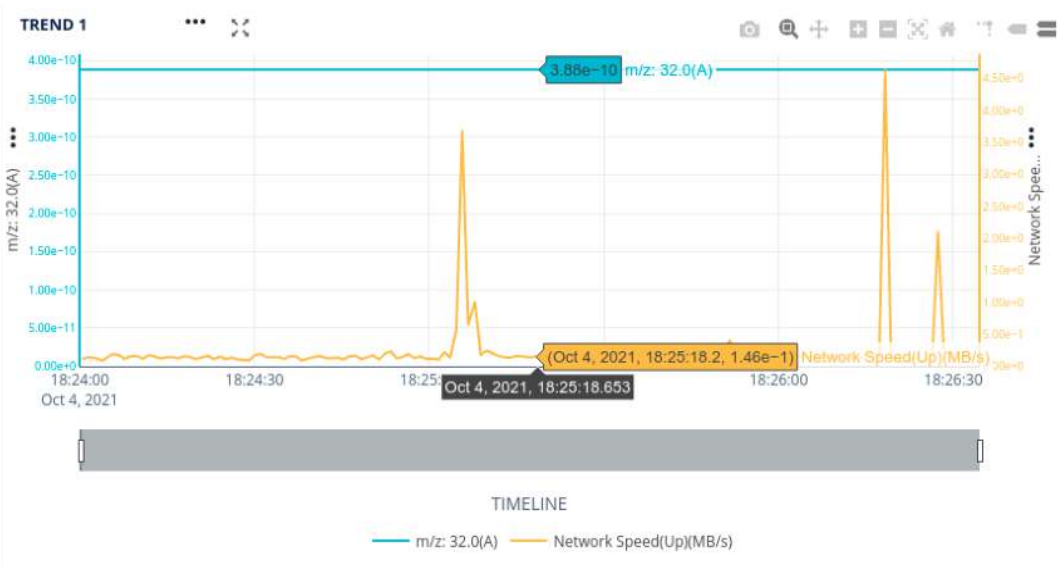
Correction algorithms can be applied on the scan trends. Users can select base correction as a data point. Users can select the multiple data points and can check the residual corrections. Users can click on display residual correction and can see the residual correction between the markers.

1.7.5.1 Steps to add residual correction factor

1. Go to the Scan page and select the trend plot which has at least one signal on it.



2. Hover cursor on plots and select a value where marker must be placed.

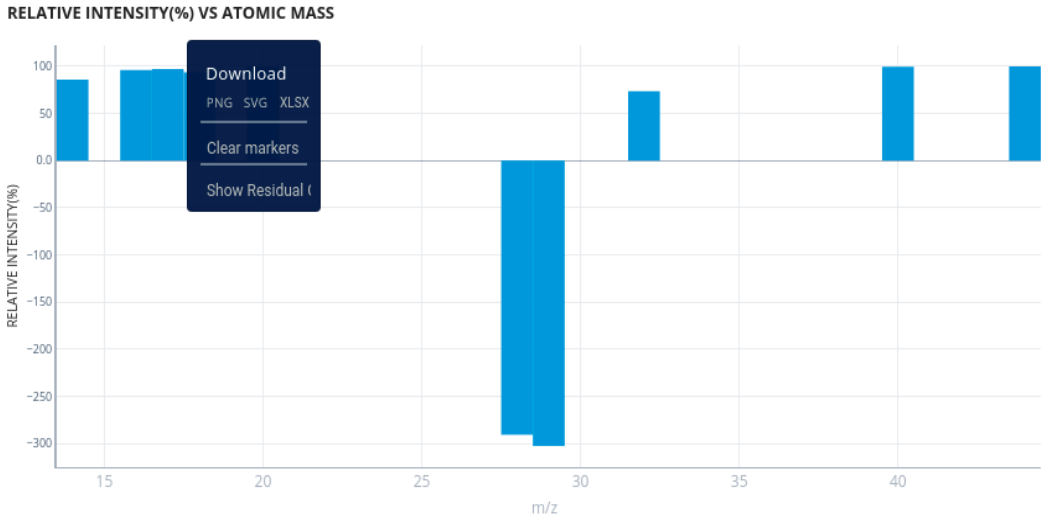


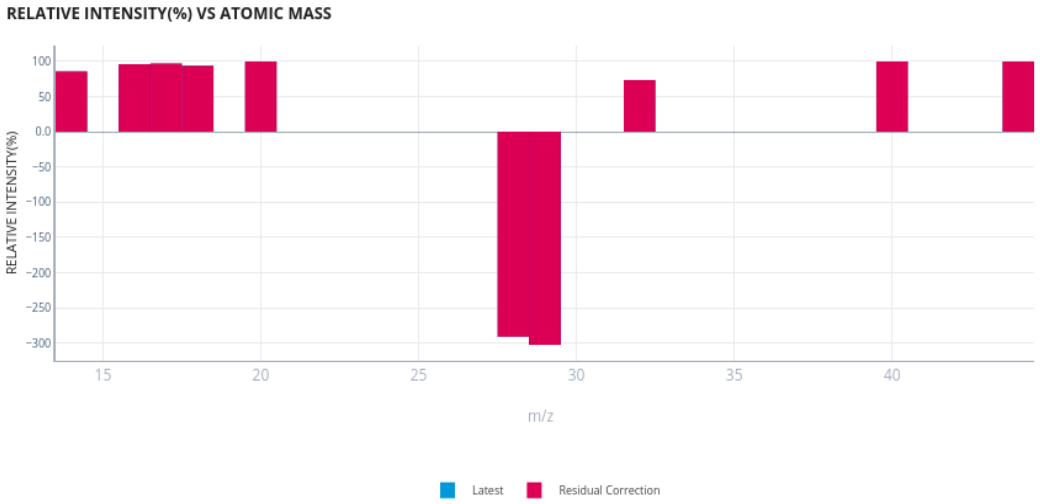
3. Add one or more markers on the trend plot by clicking at multiple points on the charts. The corresponding signals are added in the spectrum plot as shown.

4. Click on legend of the trace which has to be marked as 'Residual Correction'. On click of legend, a box will appear as below. Click on 'Mark as Residual Correction'

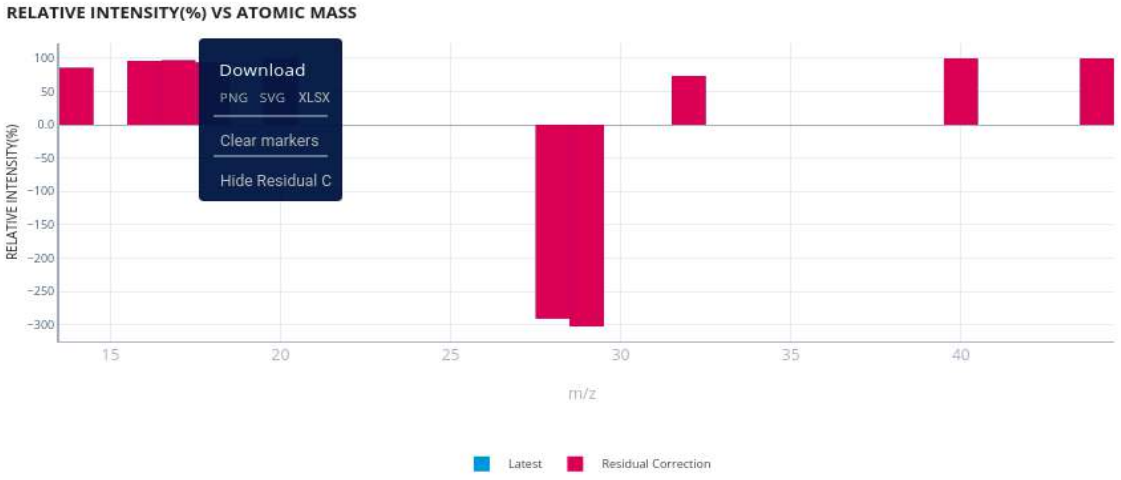
1.7.5.2 Hide or view the existing residual correction factor

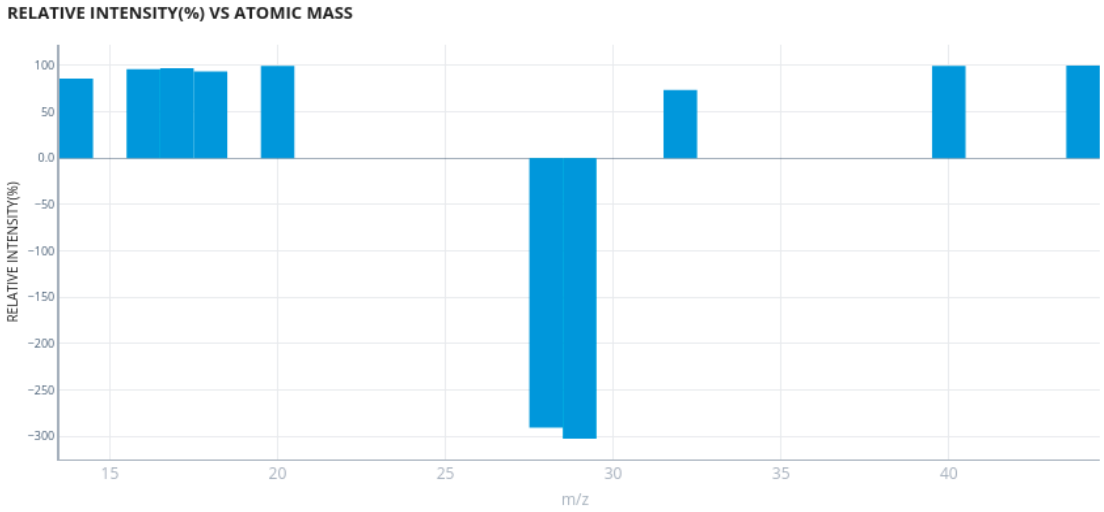
1. Click on axis-settings and select ‘Show Residual Correction’. The signal with name ‘Residual Correction’ will be added to the spectrum plot as shown.





2. Click on axis-settings and select ‘Hide Residual Correction’. The signal with name ‘Residual Correction’ will be removed from the spectrum plot as shown.





1.7.5.3 Remove the residual correction factor

Click on the legend that is marked as residual correction factor. Click on ‘Remove residual correction’

1.7.5.4 Update the residual correction factor

Click on the legend that should be updated as residual correction factor. Click on ‘Update as residual correction’

1.7.5.5 Effects of residual correction factor on plots

- All plots (Relative intensity vs atomic mass and trend plots) update its ion_current values. Updated ion_current value at a given mass 'm' is calculated as: actual_ion_current at 'm' - Residual correction factor at 'm'
- On trend plots, ion_currents values get updated only 'Ion Mass' and 'Molecule' signal type.
- The above behavior holds good in both reports and scan page.
- Partial pressure calculation will use original ion current

1.7.5.6 Residual correction factor views in reports

Downloaded scan reports

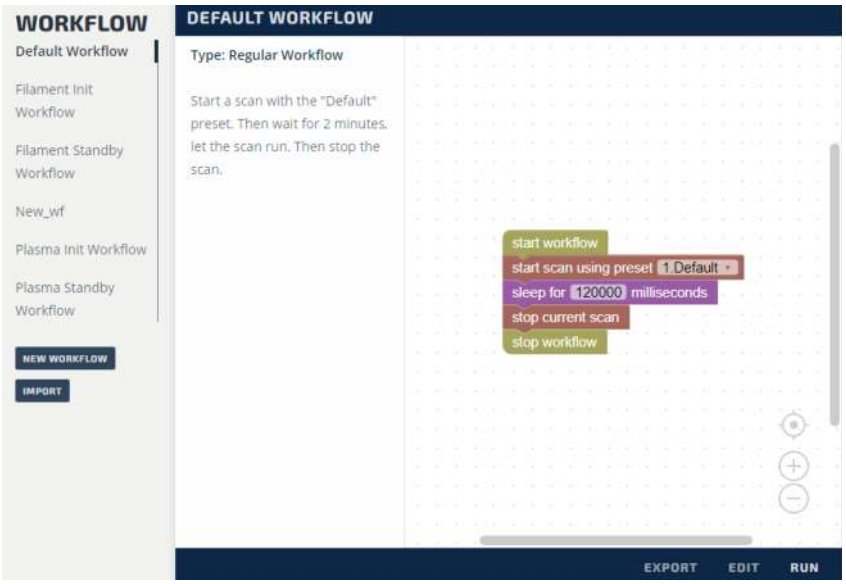
- A new sheet named 'Residual Correction' will be added in reports which consists of the selected residual factor's masses and its corresponding ion_current value
- The 'Measurements (Ion Current)' sheet consists of updated ion_currents value whenever residual correction factor is selected. Similar to plots, updated ion_current value at a given mass 'm' is calculated as: actual_ion_current at 'm' - Residual correction factor at 'm'

Live streamed reports (csv files)

- These values remain unaffected irrespective of whether residual correction factor exists or not exists. Live streamed files will always consist of actual ion-current values.

1.8 Workflow

Workflows are a visual programming feature to allow users to customize the instrument and adapt it extensively to application needs. Typical programming constructs like loops, conditional statements, arithmetic operators, variable management etc. are provided to empower the user.

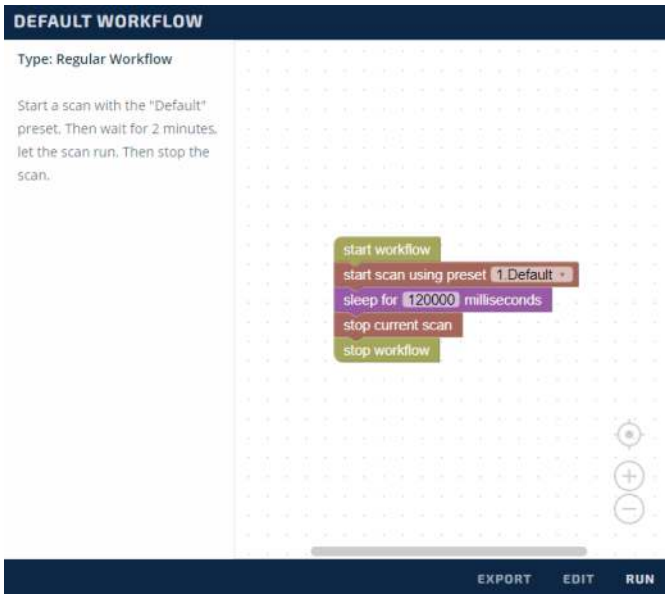


1.8.1 Workflow presets

Workflow sequences can be created and saved as a preset. Users can then run any workflow preset from the Dashboard or directly from the workflow page.

1.8.2 Edit workflow

In the edit mode, the user can modify existing sequences for execution. Programming constructs can be dragged and added to create a sequence visually.



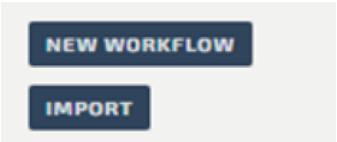
1.8.3 Run workflow

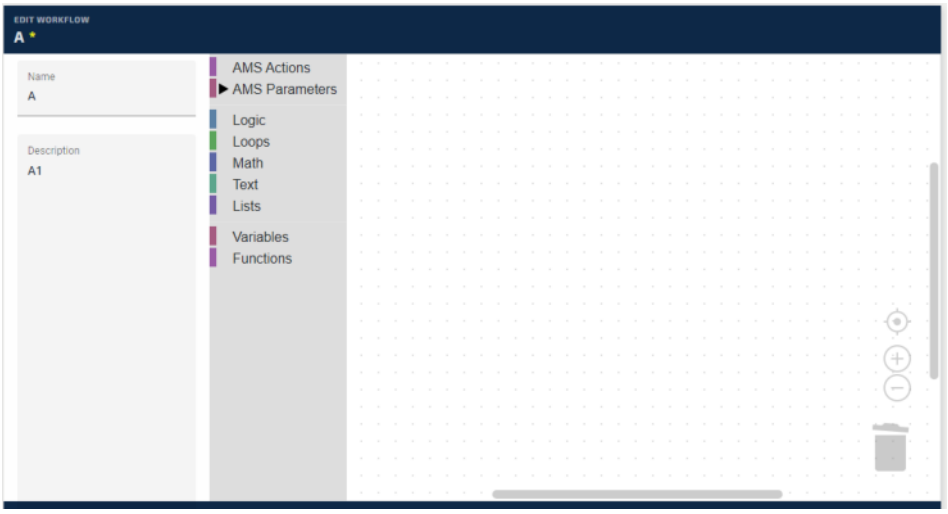
When a workflow is run, the user interface shows the current running workflow step alongside charts and other workflow related properties.

1.8.4 New Workflow

Users can create a customized workflow. Users can provide their own name and description to the workflow and import the saved workflows through the import option.

New workflow can be accessed through Navigation icons >> Workflow >> New workflow >>Name >> Description.



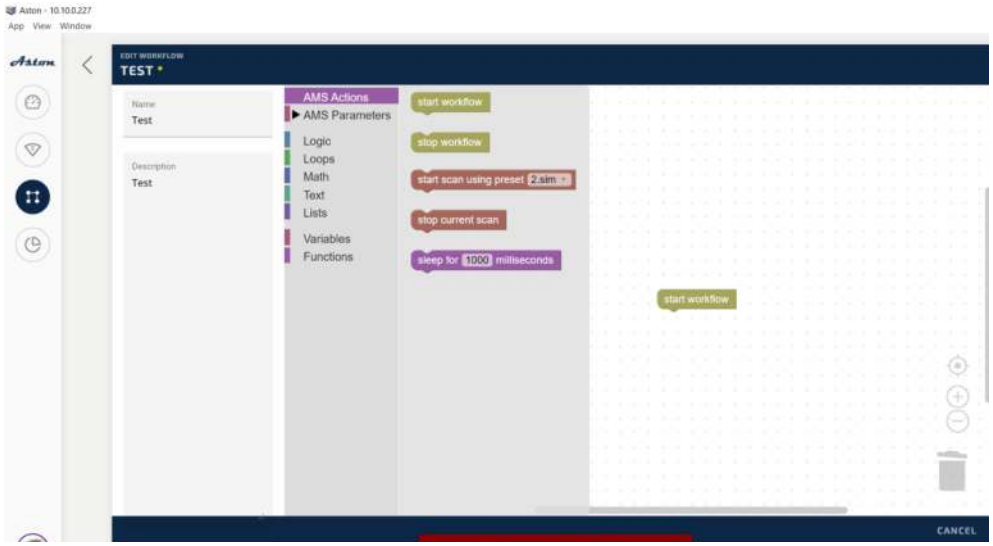


While creating the new workflow user has the option to select the type of work i.e., Regular workflow, Init workflow and standby Workflow.

Navigation icons >> Workflow >> New workflow >> Type >> Choose type of work flow.

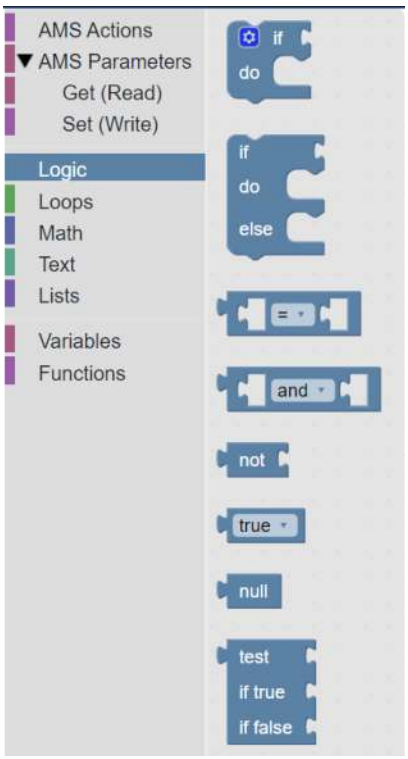
In the Aston Impact Actions, there are options to

1. Start a scan using a specific preset
2. Stop the active scan
3. Sleep (workflow will stay idle for specified milliseconds)

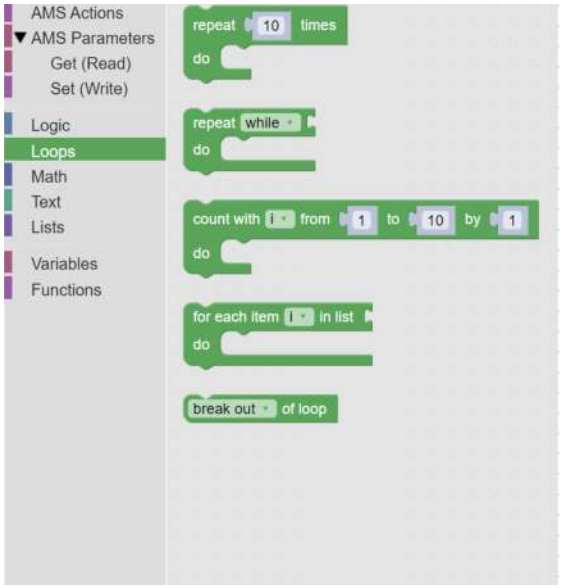


The AMS parameters have options to Read parameters (like filament status, Filament current, filament voltage status etc.) whereas Write parameters have the option to set/change the parameters.

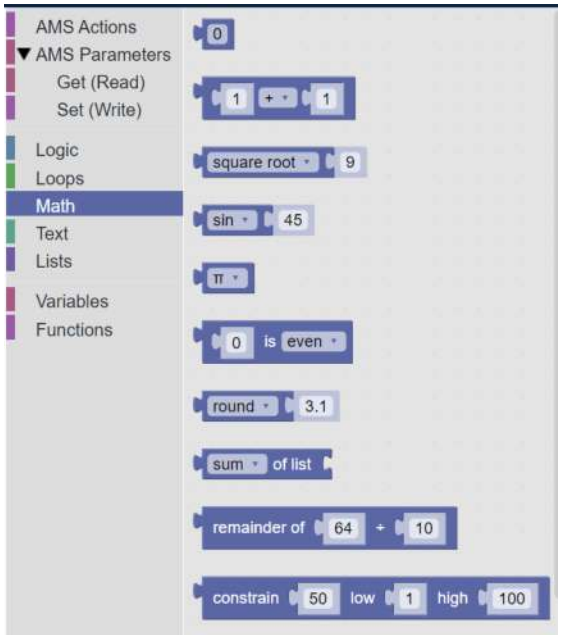
Example: Users can set filament on/off to true or false. Similarly, users can choose the filament option, filament voltage, ignition etc.
Logic parameter allows user to apply the Conditionals like "if", "if-else" and perform Logical comparisons: "==", "!=", "<", ">", etc. and Logical operations: "and", "or", "not" etc.



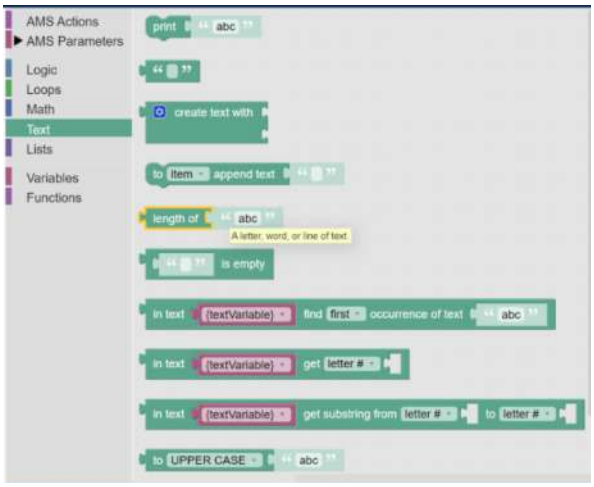
Loops parameter allows the user to perform Loop functions: "while", "for", etc.



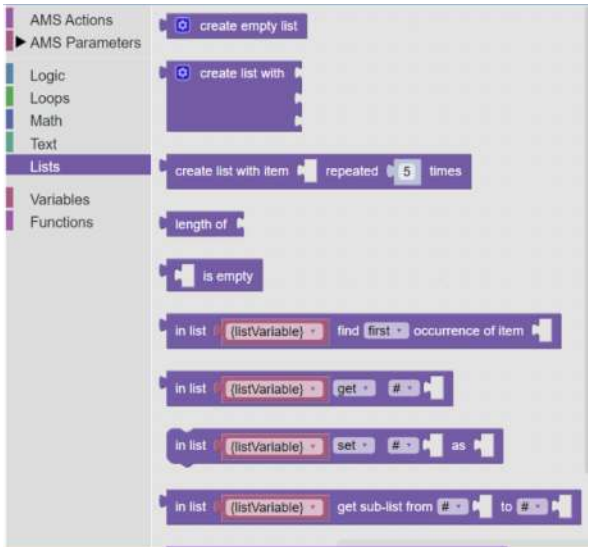
Math parameter allows user to perform the mathematical operations "+", "-", "*", square root, etc.*



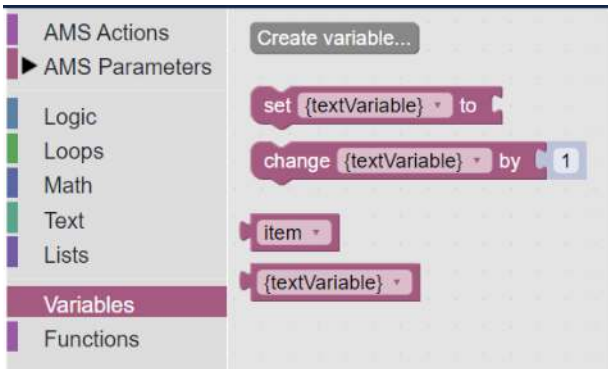
Text parameter allows the user to print/insert the text.



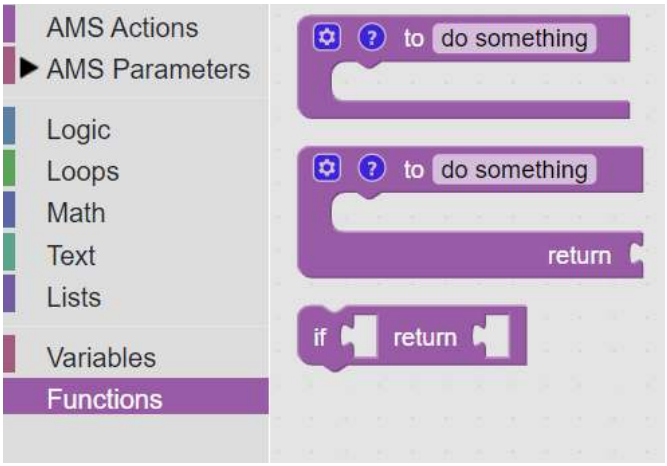
Lists parameters allow users to create the list.



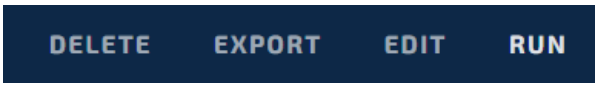
Users can create, set, and change the variable through variable parameters.



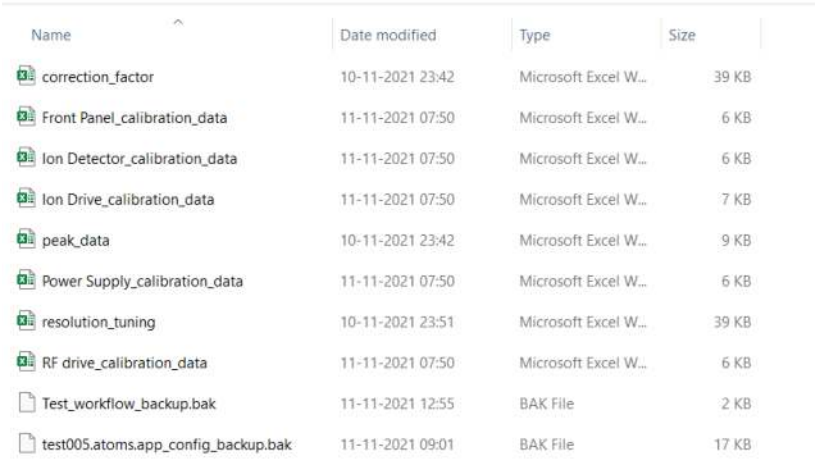
In the Function parameter, users can use the function blocks to create the functions.



The user created workflow can be saved. Users can Delete, Export, edit and run the saved workflow.



The exported workflow will be saved in the Aston Impact local folder with the same file name which the user has created. The format of the file will be .bak.



Name	Date modified	Type	Size
correction_factor	10-11-2021 23:42	Microsoft Excel W...	39 KB
Front Panel_calibration_data	11-11-2021 07:50	Microsoft Excel W...	6 KB
Ion Detector_calibration_data	11-11-2021 07:50	Microsoft Excel W...	6 KB
Ion Drive_calibration_data	11-11-2021 07:50	Microsoft Excel W...	7 KB
peak_data	10-11-2021 23:42	Microsoft Excel W...	9 KB
Power Supply_calibration_data	11-11-2021 07:50	Microsoft Excel W...	6 KB
resolution_tuning	10-11-2021 23:51	Microsoft Excel W...	39 KB
RF drive_calibration_data	11-11-2021 07:50	Microsoft Excel W...	6 KB
Test_workflow_backup.bak	11-11-2021 12:55	BAK File	2 KB
test005.atoms.app_config_backup.bak	11-11-2021 09:01	BAK File	17 KB

Users can run the created workflow. During the process the user can add notes, abort the scan and can pause the scan. During the scan process the live streaming scan data will be saved to Aston Impact local folder.

Load, save, delete, edit, copy workflows saved into the database.
Users can monitor workflow progress as it is being executed: shows which block is currently running. Abort workflow (automatically stops any active ongoing scan).

Custom designed Blockly Blocks

- The custom designed blocks offer control and monitoring of the Aston. These are all defined in ams_blocks.js, which is generated using automation
- "Start workflow" block sets up the runtime and initializes gRPC connections so that subsequent blocks can run readily
- "Start scan" block is not configured with any preset by default
    - Whenever the Workflow WebUI is loaded, a fresh list of presets is retrieved from the database and is injected into the drop-down options of this block
    - Whenever the Workflow Executer is about to launch a workflow, a fresh list of presets is retrieved from the database and is injected into the drop-down options of this block
- The blocks which fetch the values of monitored parameters from the AMS are auto-generated based on data from AmsTuple spreadsheet
- The blocks which set the values of control parameters on the AMS are auto-generated based on data from AmsTuple spreadsheet
- The custom blocks also have their Python conversions

Blockly Framework

- Blockly provides the simple drag-and-drop based UI to construct a program in a graphical way
- It comes included with general-purpose blocks like
    - Conditionals: "if", "if-else", etc.
    - Loops: "while", "for", etc.
    - Logical comparisons: "==", "!=", "<", ">", etc.
    - Logical operations: "and", "or", "not"
    - Mathematical operations: "+", "-", "*", etc.*
    - Function blocks which can be used to create functions

- It comes included with Python conversions of the included blocks also

Workflow WebUI

- Offers the ability to
    - Browse/Load saved workflows
    - Create workflows, and assign names and descriptions
    - Get warnings about problems/flaws in a workflow, from the Workflow Validator
    - Execute workflows
    - Monitor workflow activity while it is being executed: currently running block pulsates/flashes.
    - Abort workflow (automatically stops any active scan)
    - Pause/Resume workflows (not implemented yet)
- Implemented in AngularJS using components and services
- Automatically saves and restores the UI state, so that unsaved changes are not lost when the component is destroyed

Workflow Validator

- Detects problems/flaws in a workflow
- Integrated with the Workflow WebUI and runs live
- A non-exhaustive list of checks performed can found in the "Features" section at the top

Workflow Storage

- Uses TimescaleDB for storage of workflows
- The relevant schemas can be found in the DbDiagram: https://dbdiagram.io/d/5d80e7dd14d7fc1c039e0f16

Workflow Executor

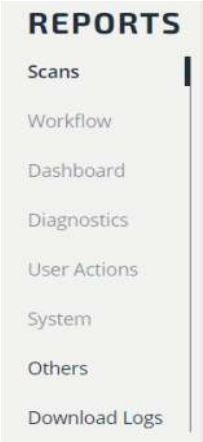
- Does not accept any Python code from the WebUI, to prevent execution of invalid/malicious code
- Accepts only a workflow ID and generates the final Python program on server itself
- A child process is spawn in which the workflow is executed
- Captures the stdout and stderr outputs of the workflow
- A child-parent pipe is used for IPC:
    - Information about currently running block

Python Final Program

- Contains the appropriate instructions to leverage the gRPC API as SDK and perform what was specified in the workflow
- Launched by the server by spawning a child process in which the Python program is executed

1.9 Reports

Users can view and export information from the Aston Impact system from the reports page.



1.9.1 Scan report

There are two kinds of scan report that are available from Aston Impact

1.9.1.1 Live Streaming Report

As soon as the scan is started the Aston Impact UI starts to download the scan report data in csv format. This report is placed under the Aston Impact-live-dump directory under the user's home directory.

	A	B	C	D	E	F	G
1	SW version:						
2	Controller SW	Plasma controller SW	IO Box SW	RF firmware	Ion Drive firmware		
3	0.9.2	Emulator	- Not Available -	- Not Available -	0.9.2		
4							
5	Hardware version:						
6	Board Name	Part Number	Serial Number	Revision Number	Calibration Date		
7	Power Supply	0	0	0	0		
8	Ion Drive	0	0	0	0		
9	Ion Detector	0	0	0	0		
10	RF drive	0	0	0	0		
11	Front Panel	0	0	0	0		
12							
13	AMS settings:						
14	Hostname	DC Minus Voltage	Voltage ramp bottom ignore	Background masses to scan for non range masses	TIA FC Slope Range 2 CB2	TIA FC Gain Range 2	Zero-blast correction end mass
15	mayer-HF.atoms.app	75	0	[10, 15, 20]	4E-07	1	6
16							
17	Scan properties:						
18	Scan ID	Scan Start Time	Measurement Type				
19	1	2022-02-16 06:19:07	Ion Current(A)				
20							
21	Scan settings:						
22	Scan preset	Description	Scan type	Ion Source	Masses to scan	Emission Current	Filament Coarse DAC
23	Quick Scan		SIM	Filament 1	[{mass:1-100,step:0.1,dwellTime:40}]	400	0
24							
25	Iteration	Time Stamp (HH:mm:ss.SSS Z)	Relative Time (HH:mm:ss.SSS)	Time for scan(ms)	Total Ion Sum	Chamber Pressure(Pa)	1
26	1	06:19:48.473 +00:00	00:00:41.209	41209	0	0.000500000023749	3.57665287899814E-10
27	2	06:20:29.024 +00:00	00:01:21.760	40551	0	0.000500000023749	3.57665287899814E-10
28	3	06:21:09.591 +00:00	00:02:02.327	40567	0	0.000500000023749	3.57665287899814E-10
29	4	06:21:50.153 +00:00	00:02:42.889	40562	0	0.000500000023749	3.57665287899814E-10
30	5	06:22:30.713 +00:00	00:03:23.449	40560	0	0.000500000023749	3.57665287899814E-10
31	6	06:23:11.276 +00:00	00:04:04.012	40563	0	0.000500000023749	3.57665287899814E-10
32	7	06:23:51.854 +00:00	00:04:44.590	40578	0	0.000500000023749	3.57665287899814E-10
33	8	06:24:32.391 +00:00	00:05:25.127	40537	0	0.000500000023749	3.57665287899814E-10
34	9	06:25:12.930 +00:00	00:06:05.666	40539	0	0.000500000023749	3.57665287899814E-10
35	10	06:25:53.461 +00:00	00:06:46.197	40531	0	0.000500000023749	3.57665287899814E-10
36	11	06:26:34.010 +00:00	00:07:26.746	40549	0	0.000500000023749	3.57665287899814E-10

1.9.1.2 Scan Report

Record of all scans performed on the system. This includes report properties, Aston settings, scans properties, and acquired spectral data.

	Iteration	Time Stamp (HI	Relative Time (HH:	Time for scan	Annotations	Total Ion Sum	Chamber Pressure(Pa)	1	1.1	1.2	1.3
2	1	16:26:42.843	00:00:41.706	41706			0.000456895	9.64E-09	9.69E-09	9.51E-09	1.73E-08
3	2	16:27:23.680	00:01:22.543	40837			0.000459242	1.52E-08	1.01E-08	1E-08	1.78E-08
4	3	16:28:04.517	00:02:03.380	40837			0.000464653	1.5E-08	9.86E-09	9.91E-09	1.75E-08
5	4	16:28:45.354	00:02:44.217	40837			0.000459242	1.49E-08	9.95E-09	9.71E-09	1.75E-08
6	5	16:29:26.191	00:03:25.054	40837			0.000446315	1.5E-08	1E-08	9.82E-09	1.79E-08
7	6	16:30:07.027	00:04:05.890	40836			0.00046194	1.51E-08	1E-08	9.91E-09	1.79E-08
8	7	16:30:47.864	00:04:46.727	40837			0.000470128	1.53E-08	1.03E-08	1.02E-08	1.85E-08
9	8	16:31:28.701	00:05:27.564	40837			0.000467383	1.54E-08	1.04E-08	1.04E-08	1.88E-08
10	9	16:32:09.538	00:06:08.401	40837			0.000470128	1.54E-08	1.05E-08	1.03E-08	1.88E-08
11	10	16:32:50.375	00:06:49.238	40837			0.000467725	1.57E-08	1.08E-08	1.07E-08	1.95E-08
12	11	16:33:31.212	00:07:30.075	40837			0.000473236	1.56E-08	1.07E-08	1.06E-08	1.93E-08
13	12	16:34:12.049	00:08:10.912	40837			0.000462278	1.59E-08	1.11E-08	1.09E-08	1.97E-08
14											

1.9.1.3 Reports listing

In option 5 (Download) - Reports can be downloaded to the user's system in MS excel format when a scan is not under execution.

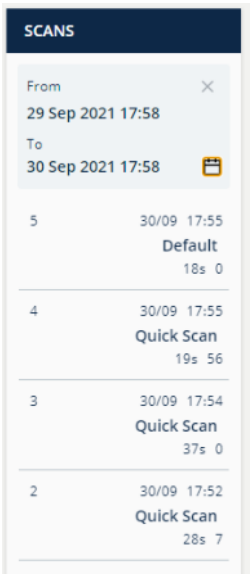
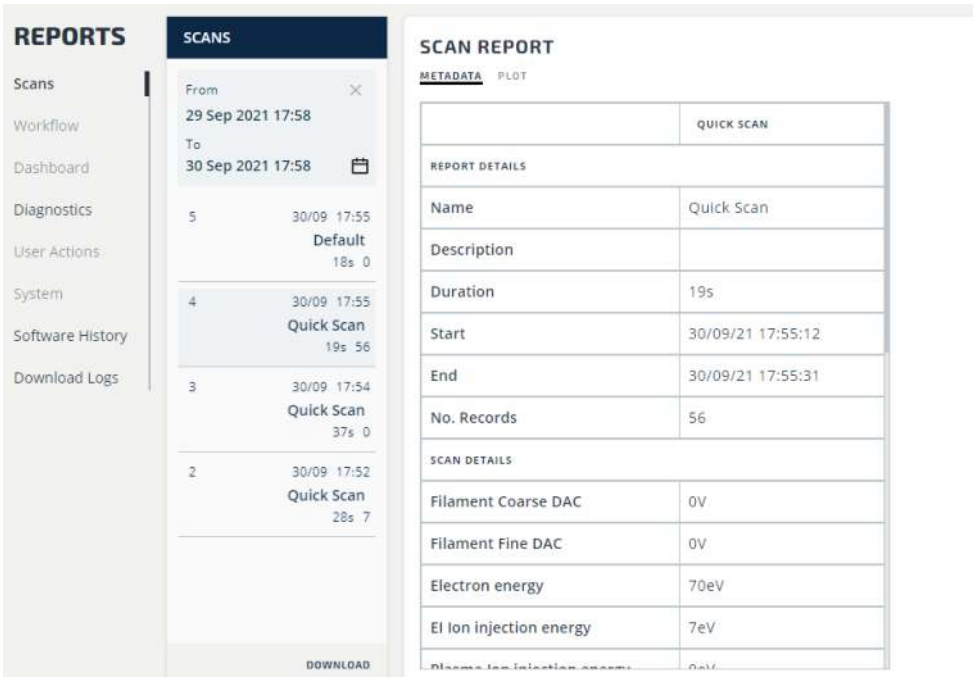


Table 33. Report listing parameters

NUMBER	PARAMETER	DESCRIPTION
1	Serial	The serial number is global run scans ID that increments through scan executions.
2	Start date-time	Date and time at which scans were run.
3	Name	A report name post fixed with a serial number. The default name is the name of the scan preset. It can be edited by the user.
4	Number of records	Total count of scan iterations run.
5	Download	Reports can be downloaded to the user's system in excel XLSX format

1.9.1.4 Metadata

The user can select a report and visualize the properties of a scan record in the metadata tab before choosing to visualize or download the report.

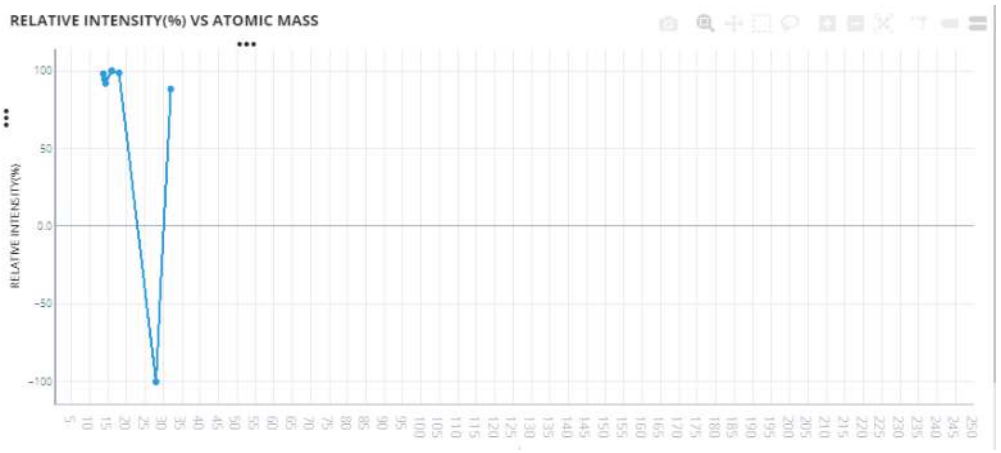


1.9.1.5 Plots

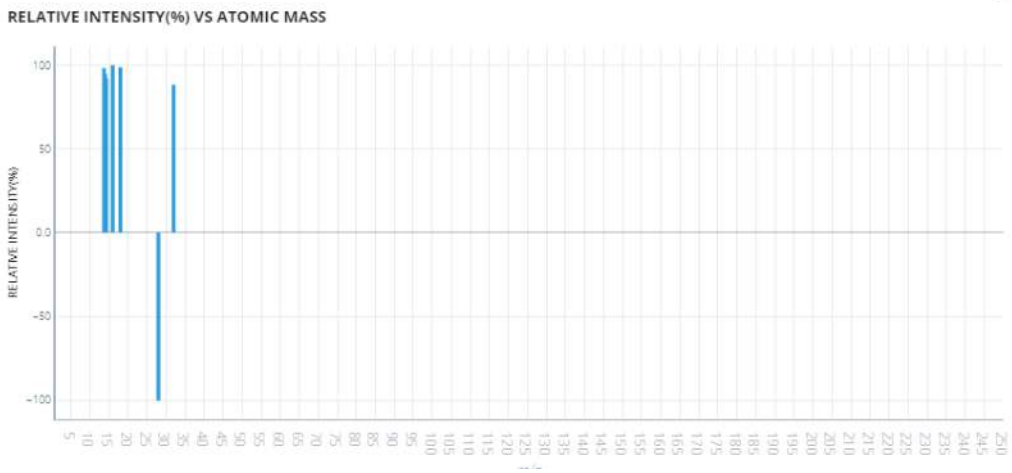
The user can visualize the data acquired from a scan record. Users can visualize different views in a single graph.

Report plots cannot be visualized when scan/workflow is running.

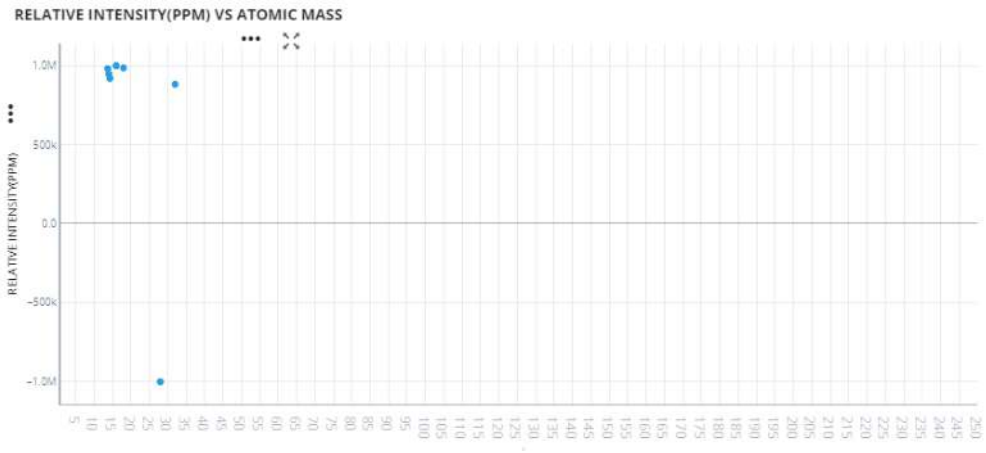
Line Graph



Bar Graph



Scatter Graph



1.9.1.6 Downloaded scan report templates

A scan report downloaded in XLSX format has multiple tabs of data to capture information. The downloaded scan reports are stored in the Aston Impact-reports folder.

a) Metadata: Captures properties of the system and configurations with which the data was acquired. For e.g. Report properties, System settings, scan properties etc.

b) Meas (Ion Cur(A)): Spectral data acquired from the running scan

c) Meas (BG-Ion Cur(A)): Background/baseline data used to correct obtained spectrum for accurate signal estimations

d) Debug Scan: Special scan mode logging internal system parameters to facilitate troubleshooting issues.

1	**Report properties:**							
2	**Report name:**	**Report description:**	**Report duration:**	**Report start time:**	**Report end time:**	**No of records in report:**	**Report Notes:**	
3	Quick Scan		8 minute 35 second 870 mill	2022-02-16 16:26:01.326	2022-02-16 16:34:37.007	12		
4								
5	**SW version:**							
6	**Controller SW**	**Plasma controller SW**	**IO Box SW**	**RF firmware**	**Ion Drive firmware**			
7	v0.9.2	v0.9.2	0.9.2	0.9.2	0.9.2			
8								
9	**Hardware version:**							
10	**Board Name**	**Part Number**	**Serial Number**	**Revision Number**	**Calibration Date**	**Time Stamp**		
11	Power Supply	0	0	0	0			
12	Ion Drive	0	0	0	0			
13	Ion Detector	0	0	0	0			
14	RF drive	0	0	0	0			
15	Front Panel	0	0	0	0			
16								
17	**AMS settings:**							
18	**Mass calibration 3rd order**	**Mass calibration 2nd order**	**Mass calibration slope**	**Mass calibration intercept**	**RF frequency**	**RF frequency search iterati**	**Maximum mass range**	**Quadrupole field radius**
19			1		3.56021623	10	250	0.0013266
20								
21	**Scan properties:**							
22	**Scan ID**	**Total scan iterations**						
23	51	12						
24								
25	**Scan settings:**							
26	**Scan preset**	**Description**	**Scan type**	**Ion Source**	**Masses to scan**	**Emission Current**	**Filament Coarse DAC**	**Filament Fine DAC**
27	Quick Scan		SIM	Filament 1	[{"mass":"1-100","step":"0.1	400.0	0	0
28								
29								
30								

MetaData | Meas (Ion Cur(A)) | Meas (BG-Ion Cur(A)) | Debug Scan

1.9.2 Dashboard report

Users can download or visualize trends of signals monitored and captured by the system. It is now disabled in the user interface.

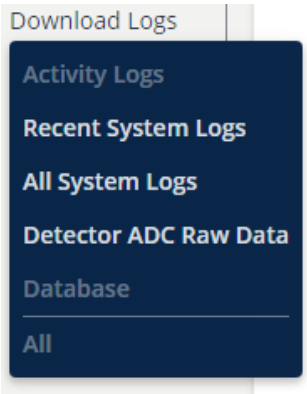
1.9.3 Diagnostics

This would let the user download the diagnostic test reports that were executed on the Aston Impact system.

1.9.4 Software History

1.9.5 Download logs

Users can download Debug Logs from the system. These logs are important as it helps to user for analysis & troubleshooting



2. ABBREVIATIONS

A	Amperes (current)
Amu	Atomic Mass Unit
BSD	Berkeley Software Distribution
CLI	Command Line Interface
COMM	Communication Port
CTS	Clear to Send
Da	Dalton
dB	Decibel
DB	Database
DC	Direct current
DHCP	Dynamic Host Configuration Protocol
DNS	Domain Name System
EI	Electron Ionization
EHS	Environmental Health and Safety
eV	Electron volt
GND	Ground
GPL	General Public License
HTTPS	Hypertext Transfer Protocol Secure
Hz	Hertz (frequency)
IP	Internet Protocol
IPv4	Internet Protocol version 4
I2C	Inter Integrated Circuit Communications
JPEG	Joint Photographic Experts Group
JSON	JavaScript Object Notation
LED	Light emitting diode
m/z	Mass to charge
Nmtui	NetworkManager Text User Interface
PC	Personal Computer
PDF	Portable Document Format

pF	Picofarads
PNG	Portable Network Graphics
RF	Radio Frequency
RPM	Revolutions per Minute
RS-232	Recommended Standard no. 232
RTS	Request to Send
RX	Receive
SoC	System on a Chip
SSH	Secure Shell
SSL	Secure Sockets Layer
SVG	Scalable Vector Graphics
Th	Thomson
TLS	Transport layer security
TTL	Transistor-Transistor Logic
TX	Transmit
U	Unified Atomic Mass Unit
USB	Universal Serial Bus
UI	User Interface
URL	Uniform Resource Locator
V	Volts (voltage)
W	Watts (power)

3. QUICK ACCESS TO ASTON IMPACT FILES

Quick Links to Aston Impact Source Files

1	Atonarp knowledge base
2	Aston Impact Windows client application
3	Aston Impact Ubuntu client application

4. GLOSSARY

Ambient Temperature

Ambient temperature is the temperature of the air surrounding a component.

Analyte

Analyte is a substance whose chemical constituents are being identified and measured.

Annotate

Annotate is technique to describe or add additional comments, notes, explanations, or other types of remarks to a plot.

Aston Impact

Aston Impact uses mass spectrometry to quantify the composition of constituents in a gas blend by measuring the mass to charge ratio of the ions generated from the blend.

Aston Impact configuration

Aston Impact configuration sets the mass spectrometer properties.

Aston Impact manager

A middleware layer of the Aston Impact software stack.

Background scan

A background scan measures the contribution of ion leakages and environment to the generated spectrum.

Baud

Baud is a component that determines the speed of communication over a data channel.

Blend

Blend is a mixture of different analyte molecules. Known blends are used for calibrating the Aston Impact.

Calorific value

The amount of energy produced by the complete combustion of a specified quantity of material or fuel.

Compliance

Following certain accepted standards

Dashboard

Dashboard is the primary page for the user to interact with and monitor the Aston Impact.

Detector

Detector is a component in the mass spectrometer which generates an electronic signal proportional to the number of ions striking it.

DHCP server

DHCP server is a network server that automatically assigns an IP addresses and other network configuration parameters to a device on a network so it can communicate with other IP networks. It relies on the standard protocol known as Dynamic Host Configuration Protocol (DHCP).

Ethernet

A system for connecting computer systems to form a local area network, to transmit the data bits containing any sort of information.

Faraday cup

Faraday cup is a component in the mass spectrometer, also known as Detector.

Filter

Filter is a process which removes or separates unwanted components. The Aston Impact requires one filter at the inlet to keep out undesired contamination.

Initialize

Bring the system into a state ready for data acquisition.

Ion Current

An ion current is the rate of flow of electrical charge associated with the flow of ions into the ion detector (electrometer/collector).

Ion source

Ion source is a component in the mass spectrometer where ionization of the analyte takes place by electron bombardment.

Ionization

Ionization is a technique used in mass spectrometer to ionize the analyte.

Mass Filter

Mass filter separates ions according to their mass-to-charge ratio (m/z).

Mass spectrometer

Mass spectrometer is an analytical technique that ionizes a sample based on their mass-to-charge ratio of the ions generated from the sample.

Molecules

A molecule is an electrically neutral group of two or more atoms held together by chemical bonds. Molecules are distinguished from ions by their lack of electrical charge.

Quadrupole

Quadrupole is a type of mass filter used in mass spectrometry. It consists of four cylindrical rods mounted in a ceramic collar. Every pair of opposing rods is electrically shorted, and a radio frequency (RF) voltage with a DC offset voltage is applied between one pair of rods and the other. The magnitude of the RF voltage determines the mass-to-charge ratio of the ions that pass through the mass filter and reach the detector. The ratio of DC-to-RF voltage determines the resolution (widths of the mass peaks).

RF to DC ratio

Ratio of the RF (AC) voltage to the DC voltage applied to the quadrupoles of a mass filter. The RF-DC ratio determines the resolution (inverse to sensitivity) of the peaks in a mass spectrum.

Scan

Each sequence of processing the ions in the mass filter followed by analysis of the ions in the detector is called a scan.

Scan configuration

Scan configuration provides options to configure the masses scanned, the number of scans run, trade- off between speed and accuracy.

Scan report

Record of all scans performed on the system. This includes system settings, mole fractions, and ion currents for all masses that are scanned.

Spectrum

Distribution of ion currents corresponding to ion fragment masses of interest.

Standby

Put the system in a state not ready for scan so that it can then be shutdown. Also required before certain features in the Aston Impact software can be used.

Workflow

Workflows allow the user to sequence scan events with unique scan properties and controls valves alongside running scans in the sequence.

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