

# MS DATA acquisition on Qtrap 5500/6500

- Open the Analyst software from the desktop.( Double click)
- Wait for some time for the software to respond.
- One window will pop up for password (password is Qtrap5500\$)
- Next Window will open

# Click on the hardware configuration

The image shows the Analyst software interface. The top menu bar includes File, Edit, View, Tools, Window, Script, and Help. Below the menu bar is a toolbar with various icons and a dropdown menu set to 'Configure Mode'. The main window displays a tree view under the 'Configure' menu. The 'Hardware Configuration' option is highlighted with a red circle. Other options in the tree include Security Configuration, Report Template Editor, Tune and Calibrate (with sub-items Compound Optimization, Instrument Optimization, and Manual Tuning), Acquire (with sub-items IDA Method Wizard, Build Acquisition Method, and Build Acquisition Batch), Explore (with sub-items Open Data File and Open Compound Database), Quantitate (with sub-items Build Quantitation Method, Quantitation Wizard, and Review Results Table), and Companion Software (with sub-items ACQUITY Console, ACQUITY Method Editor, MultiQuant 3.0.3, and Reporter 3.2).

Analyst

File Edit View Tools Window Script Help

Configure Mode Shreyas\2021\_03\_09

Configure

- Security Configuration
- Hardware Configuration**
- Report Template Editor
- Tune and Calibrate
  - Compound Optimization
  - Instrument Optimization
  - Manual Tuning
- Acquire
  - IDA Method Wizard
  - Build Acquisition Method
  - Build Acquisition Batch
- Explore
  - Open Data File
  - Open Compound Database
- Quantitate
  - Build Quantitation Method
  - Quantitation Wizard
  - Review Results Table
- Companion Software
  - ACQUITY Console
  - ACQUITY Method Editor
  - MultiQuant 3.0.3
  - Reporter 3.2

Prepared by Amrutha N., Pallavi H.U., Dr. Ankit J., Dr. Nirpendra S.

# Activate the desired profile ( For small molecule analysis with HPLC/UPLC) –select LM ( low mass 5500/6500LC)

The screenshot displays the Analyst software interface. On the left, a navigation pane lists various configuration and acquisition options. The main window shows the 'Hardware Configuration Editor' dialog box. Inside this dialog, a list of 'Hardware Profiles' is shown: 'HM 6500 LC', 'HM 6500', 'LM 6500 LC', and 'LM 6500'. The 'LM 6500 LC' profile is selected, indicated by a green checkmark and a blue highlight, and is circled in red. To the right of the list are several buttons: 'New Profile...', 'View Profile...', 'Delete Profile', 'Deactivate Profile', 'Available Devices...', 'Close', and 'Help'. The 'Close' button is also circled in red. The Windows taskbar at the bottom shows the system tray with the date and time as 09:31 on 24-11-2021.

# Hardware Configuration Editor



## Hardware Profiles:

- HM 6500 LC
  - Mass Spectrometer QTRAP 6500 (0) on Ethernet
  - Software Application ACQUITY UPLC System (0)
- HM 6500
  - Mass Spectrometer QTRAP 6500 (0) on Ethernet
- LM 6500 LC
  - Mass Spectrometer QTRAP 6500 (0) on Ethernet
  - Software Application ACQUITY UPLC System (0)
- LM 6500
  - Mass Spectrometer QTRAP 6500 (0) on Ethernet

New Profile...

View Profile...

Delete Profile

Deactivate Profile

Available Devices...

Close

Help

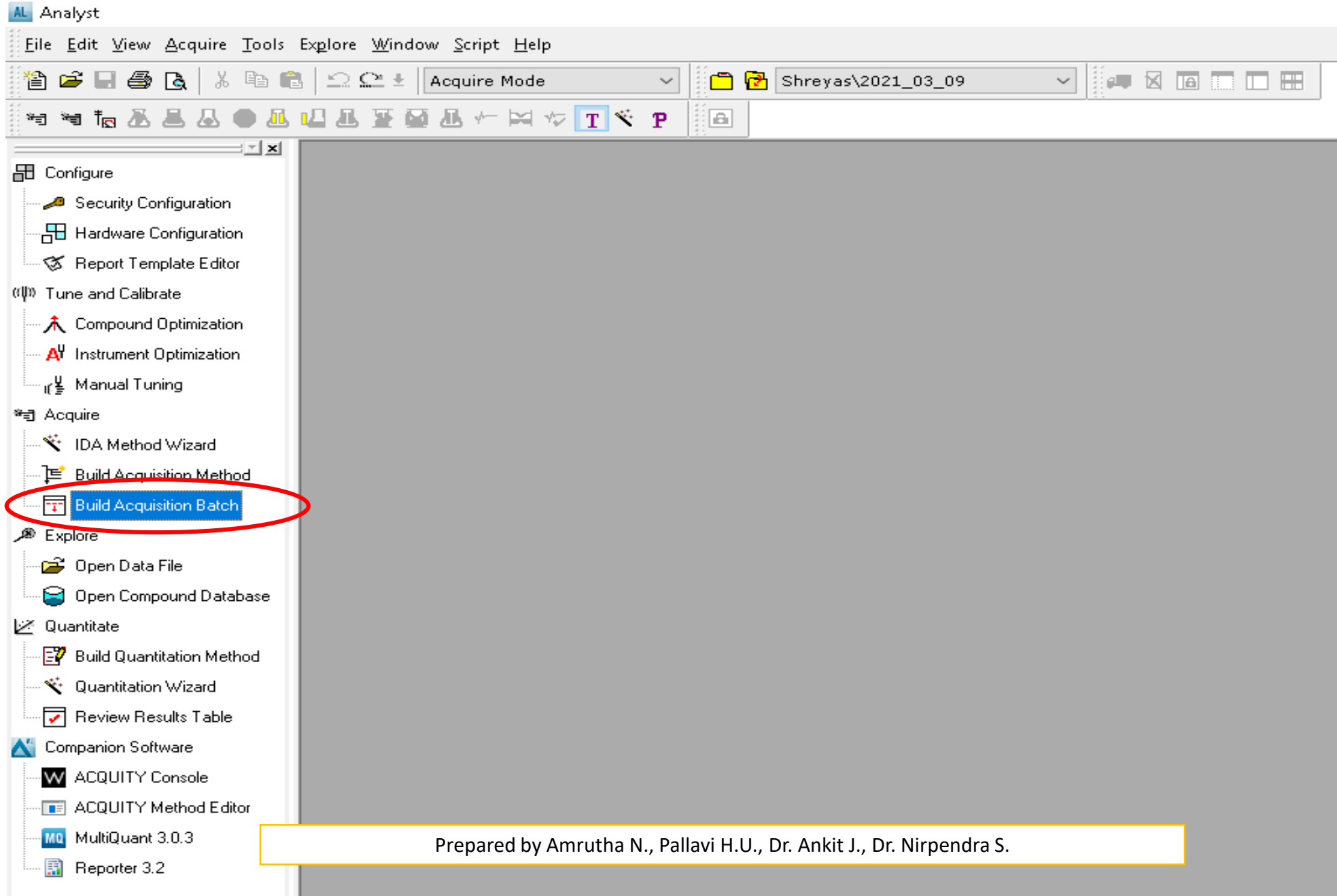


**Create your project from the tool box before starting ( for new users)  
you need to copy any method from the desired folder of your lab folder to this folder before starting.**

The screenshot displays the Analyst software interface. The 'Tools' menu is open, and the 'Project' option is highlighted. The sub-menu for 'Project' is also open, showing options such as 'Create Project...', 'Create Subproject...', 'Select/Configure...', 'Copy Project...', 'Copy Subproject...', 'Copy Data...', 'Create Root Directory...', and 'Set Root Directory...'. The interface includes a sidebar with various tool categories like 'Configure', 'Tune and Calibrate', 'Acquire', and 'Quantitate'. A data table is visible at the bottom of the interface.

Sample Name	Rack Code	Rack Position	Plate Code	Plate Position	Vial Position	Data File	Inj. Volume (µl)
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Select your desired folder and go to build acquisition batch after copying the method from the lab folder



## Once you click on the build acquisition batch-new window will open as below

Analyst - [Batch Editor: [Shreyas\2021\_03\_09 - New Batch]]

File Edit View Acquire Tools Explore Window Script Help

Acquire Mode Shreyas\2021\_03\_09

Configure

- Security Configuration
- Hardware Configuration
- Report Template Editor

Tune and Calibrate

- Compound Optimization
- Instrument Optimization
- Manual Tuning

Acquire (1)

- IDA Method Wizard
- Build Acquisition Method
- Build Acquisition Batch

Explore

- Open Data File
- Open Compound Database

Quantitate

- Build Quantitation Method
- Quantitation Wizard
- Review Results Table

Companion Software

- ACQUITY Console
- ACQUITY Method Editor
- MultiQuant 3.0.3
- Reporter 3.2

Sample Locations Quantitation Submit

Select Method for Sample Set

Set: SET1

Quantitation

none Quick Quant

Acquisition

Use as Template none Method Editor

Use Multiple Methods

Batch Script: Select Script

Sample Name	Rack Code	Rack Position	Plate Code	Plate Position	Vial Position	Data File	Inj. Volume (µl)
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Put the name of your set ( I put date in place of set name) and click on add sample button. From the method editor drop down the method of your choice, if you want to run separate method for separate run then use multiple method option should be checked.

Analyst - [Batch Editor: [Shreyas\2021\_03\_09 - New Batch]]

File Edit View Acquire Tools Explore Window Script Help

Acquire Mode Shreyas\2021\_03\_09

Configure

- Security Configuration
- Hardware Configuration
- Report Template Editor
- Tune and Calibrate
  - Compound Optimization
  - Instrument Optimization
  - Manual Tuning
- Acquire (1)
  - IDA Method Wizard
  - Build Acquisition Method
  - Build Acquisition Batch
- Explore
  - Open Data File
  - Open Compound Database
- Quantitate
  - Build Quantitation Method
  - Quantitation Wizard
  - Review Results Table
- Companion Software
  - ACQUITY Console
  - ACQUITY Method Editor
  - MultiQuant 3.0.3
  - Reporter 3.2

Sample Locations Quantitation Submit

Select Method for Sample Set

Set: 24112021

Quantitation: none Quick Quant

Add Set Remove Set

Acquisition

Use as Template

Use Multiple Methods

Method Editor

Add Samples

Batch Script: Select Script

Sample Name	Rack Code	Rack Position	Plate Code	Plate Position	Vial Position	Data File	Inj. Volume (µl)
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Sample prefix name and data file prefix name should be assigned here along with put the number of samples in new sample number ( I put one sample) you want to add to the batch.

The screenshot displays the Analyst software interface. The main window shows the 'Sample' tab with configuration options for 'Set' (24112021), 'Quantitation' (none), and 'Acquisition' (Use as Template: none, Use Multiple Methods: unchecked). A table header is visible at the bottom of the main window with columns: Sample Name, Rack Code, Rack Position, Plate Code, Plate Position, Vial Position, Data File, Inj. Volume (µl).

The 'Add Sample' dialog box is open, showing the following fields and options:

- Sample name:** Prefix: ; Sample number: ; Number of digits:
- Data file:** Prefix: ; Set name: ; Auto Increment: ; Sub Folder: ;
- New samples:** Number:

Buttons at the bottom of the dialog box are , , and .

Analyst - [Batch Editor: [Shreyas\2021\_03\_09 - New Batch]]

File Edit View Acquire Tools Explore Window Script Help

Acquire Mode | Shreyas\2021\_03\_09

Configure

- Security Configuration
- Hardware Configuration
- Report Template Editor

Tune and Calibrate

- Compound Optimization
- Instrument Optimization
- Manual Tuning

Acquire (1)

- IDA Method Wizard
- Build Acquisition Method
- Build Acquisition Batch

Explore

- Open Data File
- Open Compound Database

Quantitate

- Build Quantitation Method
- Quantitation Wizard
- Review Results Table

Companion Software

- ACQUITY Console
- ACQUITY Method Editor
- MultiQuant 3.0.3
- Reporter 3.2

Sample Locations Quantitation Submit

Select Method for Sample Set

Set: 24112021 Quantitation: none Quick Quant

Add Set Remove Set Add Samples Del Samples

Acquisition

Use as Template none Method Editor

Use Multiple Methods

Batch Script: Select Script

Sample Name	Rack Code	Rack Position	Plate Code	Plate Position	Vial Position	Data File	Inj. Volume (µl)
Blank001	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank002	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank003	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank004	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank005	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank006	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank007	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank008	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank009	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank010	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank011	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank012	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank013	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank014	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank015	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank016	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank017	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank018	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank019	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank020	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank021	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank022	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank023	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank024	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank025	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank026	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank027	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank028	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank029	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank030	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank031	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank032	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank033	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank034	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank035	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank036	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank037	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank038	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank039	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank040	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank041	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank042	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank043	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank044	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank045	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000
Blank046	Sample Manager	1	ANSI-384.well100uL	1	0	Blank2411202	-1.000

Once you click ok on the previous box, new batch will be created with desired data file prefix and sample name prefix, it is advisable to put your data file name/sample name as default setup. So that you all raw files will be stack in one folder.

# If not selected the method before you can select the method now also from method editor

The screenshot displays the Analyst software interface. The 'Sample' tab is active, showing a table of samples and a 'Select Method for Sample Set' dialog. A red circle highlights the 'Method Editor' button in the dialog. A red rectangle highlights a dropdown menu with the following options:

- SugarP\_18082021
- none
- 20210203 Sabari\_AcoA positive
- 20210903\_Shreyas\_Arg0rn
- 25022021\_AA\_NTS\_GSH
- Glycolytic13C\_ZR
- Glycolytic\_13C\_Asp
- Glycolytic\_ZR
- OBHA\_09052018
- SugarP\_18082021
- Sugarp\_NAD\_AcoA\_Shreyas\_20210108

Sample Name	Rack Code	Rack Position	Plate	Injection File	Inj. Volume (µl)
1 Blank001	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
2 Blank002	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
3 Blank003	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
4 Blank004	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
5 Blank005	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
6 Blank006	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
7 Blank007	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
8 Blank008	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
9 Blank009	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
10 Blank010	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
11 Blank011	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
12 Blank012	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
13 Blank013	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
14 Blank014	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
15 Blank015	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
16 Blank016	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
17 Blank017	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
18 Blank018	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
19 Blank019	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
20 Blank020	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
21 Blank021	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
22 Blank022	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
23 Blank023	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
24 Blank024	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
25 Blank025	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
26 Blank026	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
27 Blank027	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
28 Blank028	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
29 Blank029	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
30 Blank030	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
31 Blank031	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
32 Blank032	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
33 Blank033	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
34 Blank034	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
35 Blank035	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
36 Blank036	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
37 Blank037	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
38 Blank038	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
39 Blank039	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
40 Blank040	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
41 Blank041	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
42 Blank042	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
43 Blank043	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
44 Blank044	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
45 Blank045	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000
46 Blank046	Sample Manager	1	ANSI-384well100uL	Blank2411202	10.000

For Help, press F1

Prepared by Amrutha N., Pallavi H.U., Dr. Ankit J., Dr. Nirpendra S.

KTOP-STIHJRS\sciex D:\Analyst Data Idle Idle Ready 09:36 24-11-2021

Or you can select use multiple method and fill in the acquisition method column after selection the use multiple method

The screenshot displays the Analyst software interface. The main window is titled "Batch Editor: [Shreyas\2021\_03\_09 - New Batch]". The interface includes a menu bar (File, Edit, View, Acquire, Tools, Explore, Window, Script, Help) and a toolbar. On the left, there is a "Configure" sidebar with options like Security Configuration, Hardware Configuration, Report Template Editor, Tune and Calibrate, and Acquire (1). The central area shows a "Select Method for Sample Set" dialog box with a "Set" dropdown (24112021), a "Quantitation" dropdown (none), and an "Acquisition" dropdown (SugarP\_18082021). The "Use Multiple Methods" checkbox is checked. Below the dialog is a "Batch Script" field. The main data table lists 46 samples, each with columns for Sample Name, Rack Code, Rack Position, Plate Code, Plate Position, Vial Position, Acquisition Method, Data File, and Inj. Volume (µl). The "Acquisition Method" column for sample 1 is circled in red, showing "SugarP\_NAD\_AcoA\_Shreyas\_20210108".

	Sample Name	Rack Code	Rack Position	Plate Code	Plate Position	Vial Position	Acquisition Method	Data File	Inj. Volume (µl)
1	Blank001	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_NAD_AcoA_Shreyas_20210108	Blank2411202	10.000
2	Blank002	Sample Manager	1	ANSI-384well100uL	1	0	Glycolytic_21	Blank2411202	10.000
3	Blank003	Sample Manager	1	ANSI-384well100uL	1	0	20210903_Shreyas_ArgOrn	Blank2411202	10.000
4	Blank004	Sample Manager	1	ANSI-384well100uL	1	0	25022021_AA_NTS_GSH	Blank2411202	10.000
5	Blank005	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
6	Blank006	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
7	Blank007	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
8	Blank008	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
9	Blank009	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
10	Blank010	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
11	Blank011	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
12	Blank012	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
13	Blank013	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
14	Blank014	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
15	Blank015	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
16	Blank016	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
17	Blank017	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
18	Blank018	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
19	Blank019	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
20	Blank020	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
21	Blank021	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
22	Blank022	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
23	Blank023	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
24	Blank024	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
25	Blank025	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
26	Blank026	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
27	Blank027	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
28	Blank028	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
29	Blank029	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
30	Blank030	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
31	Blank031	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
32	Blank032	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
33	Blank033	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
34	Blank034	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
35	Blank035	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
36	Blank036	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
37	Blank037	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
38	Blank038	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
39	Blank039	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
40	Blank040	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
41	Blank041	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
42	Blank042	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
43	Blank043	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
44	Blank044	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
45	Blank045	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000
46	Blank046	Sample Manager	1	ANSI-384well100uL	1	0	SugarP_18082021	Blank2411202	10.000

# Anytime new samples can be added to the sample table by add sample button and sample name will have auto increment option in the column

The screenshot displays the Analyst software interface. On the left is a navigation pane with various tool categories. The main window is titled 'Sample' and contains configuration options for 'Set' (24112021), 'Quantitation' (none), and 'Acquisition' (SugarP\_18082021). A red circle highlights the 'Add Samples' button. Below these options is a 'Batch Script' field and a 'Select Script' button. The central part of the interface is a table with the following columns: Sample Name, Rack Code, Rack Position, Plate Code, Plate Position, Vial Position, Data File, and Inj. Volume (µl). The table lists 45 samples, starting with 'Sample1' and followed by 'Blank002' through 'Blank045'. The 'Sample Name' column shows an auto-incrementing pattern. At the bottom, a yellow box contains the text 'Prepared by Amrutha N., Pallavi H.U., Dr. Ankit J., Dr. Nirpendra S.' The Windows taskbar at the bottom shows the system tray with the date 24-11-2021 and time 09:40.

	Sample Name	Rack Code	Rack Position	Plate Code	Plate Position	Vial Position	Data File	Inj. Volume (µl)
1	Sample1	Sample Manager	1	ANSI-384well100uL	1	0	24112021\	10.000
2	Blank002	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
3	Blank003	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
4	Blank004	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
5	Blank005	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
6	Blank006	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
7	Blank007	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
8	Blank008	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
9	Blank009	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
10	Blank010	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
11	Blank011	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
12	Blank012	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
13	Blank013	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
14	Blank014	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
15	Blank015	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
16	Blank016	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
17	Blank017	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
18	Blank018	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
19	Blank019	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
20	Blank020	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
21	Blank021	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
22	Blank022	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
23	Blank023	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
24	Blank024	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
25	Blank025	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
26	Blank026	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
27	Blank027	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
28	Blank028	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
29	Blank029	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
30	Blank030	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
31	Blank031	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
32	Blank032	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
33	Blank033	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
34	Blank034	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
35	Blank035	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
36	Blank036	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
37	Blank037	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
38	Blank038	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
39	Blank039	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
40	Blank040	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
41	Blank041	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
42	Blank042	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
43	Blank043	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
44	Blank044	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
45	Blank045	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000
46	Blank046	Sample Manager	1	ANSI-384well100uL	1	0	Blank24112021	10.000

# To autofill the table in any column right click on mouse and select fill down or auto increment

The screenshot displays the Analyst software interface. The main window shows a table with columns: Sample Name, Rack Code, Rack Position, Plate Code, Plate Position, Vial Position, Data File, and Inj. Volume (µl). A right-click context menu is open over the 'Inj. Volume (µl)' column, with 'AutoIncrement' selected. The table contains 46 rows of data, all with an 'Inj. Volume' of 10.000. The software interface includes a menu bar (File, Edit, View, Acquire, Tools, Explore, Window, Script, Help), a toolbar, and a left-hand navigation pane with categories like Configure, Acquire, Quantitate, and Companion Software.

Sample Name	Rack Code	Rack Position	Plate Code	Plate Position	Vial Position	Data File	Inj. Volume (µl)
1	Blank001	Open...	NSI-384well00uL	1	0	Blank24112021	10.000
2	Blank002	Import From	NSI-384well00uL	1	0	Blank24112021	10.000
3	Blank003		NSI-384well00uL	1	0	Blank24112021	10.000
4	Blank004	Save As Batch	NSI-384well00uL	1	0	Blank24112021	10.000
5	Blank005	Save As a Template...	NSI-384well00uL	1	0	Blank24112021	10.000
6	Blank006		NSI-384well00uL	1	0	Blank24112021	10.000
7	Blank007	Hide/Show Column...	NSI-384well00uL	1	0	Blank24112021	10.000
8	Blank008	Save Column Settings...	NSI-384well00uL	1	0	Blank24112021	10.000
9	Blank009		NSI-384well00uL	1	0	Blank24112021	10.000
10	Blank010	Add Custom Column	NSI-384well00uL	1	0	Blank24112021	10.000
11	Blank011	Delete Custom Column	NSI-384well00uL	1	0	Blank24112021	10.000
12	Blank012		NSI-384well00uL	1	0	Blank24112021	10.000
13	Blank013	Fill Down	NSI-384well00uL	1	0	Blank24112021	10.000
14	Blank014	AutoIncrement	NSI-384well00uL	1	0	Blank24112021	10.000
15	Blank015		NSI-384well00uL	1	0	Blank24112021	10.000
16	Blank016	Delete Samples	NSI-384well00uL	1	0	Blank24112021	10.000
17	Blank017	Other...	NSI-384well00uL	1	0	Blank24112021	10.000
18	Blank018		NSI-384well00uL	1	0	Blank24112021	10.000
19	Blank019	Select Autosampler	NSI-384well00uL	1	0	Blank24112021	10.000
20	Blank020		NSI-384well00uL	1	0	Blank24112021	10.000
21	Blank021	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
22	Blank022	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
23	Blank023	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
24	Blank024	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
25	Blank025	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
26	Blank026	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
27	Blank027	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
28	Blank028	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
29	Blank029	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
30	Blank030	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
31	Blank031	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
32	Blank032	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
33	Blank033	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
34	Blank034	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
35	Blank035	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
36	Blank036	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
37	Blank037	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
38	Blank038	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
39	Blank039	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
40	Blank040	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
41	Blank041	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
42	Blank042	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
43	Blank043	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
44	Blank044	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
45	Blank045	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000
46	Blank046	Sample Manager	ANSI-384well00uL	1	0	Blank24112021	10.000

Prepared by Amrutha N., Pallavi H.U., Dr. Ankit J., Dr. Nirpendra S.

# Fill down the column

Analyst - [Batch Editor: [Shreyas\2021\_03\_09 - New Batch]]

File Edit View Acquire Tools Explore Window Script Help

Acquire Mode Shreyas\2021\_03\_09

Configure

- Security Configuration
- Hardware Configuration
- Report Template Editor
- Tune and Calibrate
  - Compound Optimization
  - Instrument Optimization
  - Manual Tuning
- Acquire (1)
  - IDA Method Wizard
  - Build Acquisition Method
  - Build Acquisition Batch
- Explore
  - Open Data File
  - Open Compound Database
- Quantitate
  - Build Quantitation Method
  - Quantitation Wizard
  - Review Results Table
- Companion Software
  - ACQUITY Console
  - ACQUITY Method Editor
  - MuQuant 3.0.3
  - Reporter 3.2

Sample Locations Quantitation Submit

Select Method for Sample Set

Set: 24112021 Quantitation: none Quick Quant

Add Set Remove Set

Acquisition

Use as Template SugarP\_18082021 Method Editor

Use Multiple Methods

Add Samples Del Samples

Batch Script: Select Script

	Sample Name	Rack Code	Rack Position	Plate Code	Data File	Inj. Volume (µl)
1	sample1	Sample Manager	1	ANSI-48Vial2mL.Ho	ink24112021	10.000
2	sample2	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
3	sample3	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
4	sample4	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
5	sample5	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
6	sample6	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
7	sample7	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
8	sample8	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
9	sample9	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
10	sample10	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
11	sample11	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
12	sample12	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
13	sample13	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
14	sample14	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
15	sample15	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
16	sample16	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
17	sample17	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
18	sample18	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
19	sample19	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
20	sample20	Sample Manager	1	ANSI-384well100ul	ink24112021	10.000
21	sample21	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
22	sample22	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
23	sample23	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
24	sample24	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
25	sample25	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
26	sample26	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
27	sample27	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
28	sample28	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
29	sample29	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
30	sample30	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
31	sample31	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
32	sample32	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
33	sample33	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
34	sample34	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
35	sample35	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
36	sample36	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
37	sample37	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
38	sample38	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
39	sample39	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
40	sample40	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
41	sample41	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
42	sample42	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
43	sample43	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
44	sample44	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
45	sample45	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000
46	sample46	Sample Manager	1	ANSI-384well100ul	1 0 Blank24112021	10.000

Open... Import From Save As Batch Save As a Template... Hide/Show Column... Save Column Settings... Add Custom Column Delete Custom Column Fill Down Autoincrement Delete Samples Other... Select Autosampler

For Help, press F1

P-STIHJ5R\scies D:\Analyst Data Idle Idle Ready 09:42 24-11-2021

# Fill the injection volume of your sample

Analyst - [Batch Editor: [Shreyas\2021\_03\_09 - New Batch]]

File Edit View Acquire Tools Explore Window Script Help

Acquire Mode Shreyas\2021\_03\_09

Configure

- Security Configuration
- Hardware Configuration
- Report Template Editor

Tune and Calibrate

- Compound Optimization
- Instrument Optimization
- Manual Tuning

Acquire (1)

- IDA Method Wizard
- Build Acquisition Method
- Build Acquisition Batch

Explore

- Open Data File
- Open Compound Database

Quantitate

- Build Quantitation Method
- Quantitation Wizard
- Review Results Table

Companion Software

- ACQUITY Console
- ACQUITY Method Editor
- MultiQuant 3.0.3
- Reporter 3.2

Sample Locations Quantitation Submit

Select Method for Sample Set

Set: 24112021 Quantitation: none Quick Quant

Add Set Remove Set Add Samples Del Samples

Acquisition

Use as Template SugarP\_18082021 Method Editor

Use Multiple Methods

Batch Script: Select Script

	Sample Name	Rack Code	Rack Position	Plate Code	Plate Position	Vial Position	Data File	Inj Volume (µl)
1	sample1	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	24112021\	20.00
2	sample2	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
3	sample3	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
4	sample4	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
5	sample5	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	0.000
6	sample6	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	0.000
7	sample7	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	0.000
8	sample8	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	0.000
9	sample9	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
10	sample10	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
11	sample11	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
12	sample12	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
13	sample13	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
14	sample14	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
15	sample15	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
16	sample16	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
17	sample17	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
18	sample18	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
19	sample19	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
20	sample20	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
21	sample21	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
22	sample22	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
23	sample23	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
24	sample24	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
25	sample25	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
26	sample26	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
27	sample27	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
28	sample28	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
29	sample29	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
30	sample30	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
31	sample31	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
32	sample32	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
33	sample33	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
34	sample34	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
35	sample35	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
36	sample36	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
37	sample37	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	0.000
38	sample38	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	0.000
39	sample39	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	0.000
40	sample40	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	0.000
41	sample41	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
42	sample42	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
43	sample43	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
44	sample44	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
45	sample45	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	10.000
46	sample46	Sample Manager	1	ANSI-48Vial2mLHolder	1	1	Blank24112021	20.000

For Help, press F1

Prepared by Amrutha N., Pallavi H.U., Dr. Ankit J., Dr. Nirpendra S.

TIHJ5R\sciex D:\Analyst Data Idle Idle Ready 09:44 24-11-2021



Analyst - [Batch Editor: [Shreyas\2021\_03\_09 - New Batch]]

File Edit View Acquire Tools Explore Window Script Help

Acquire Mode Shreyas\2021\_03\_09

Configure

- Security Configuration
- Hardware Configuration
- Report Template Editor
- Tune and Calibrate
- Compound Optimization
- Instrument Optimization
- Manual Tuning
- Acquire (1)
  - IDA Method Wizard
  - Build Acquisition Method
  - Build Acquisition Batch
- Explore
  - Open Data File
  - Open Compound Database
- Quantitate
  - Build Quantitation Method
  - Quantitation Wizard
  - Review Results Table
- Companion Software
  - ACQUITY Console
  - ACQUITY Method Editor
  - MultiQuant 3.0.3
  - Reporter 3.2

Sample Locations Quantitation Submit

Autosampler: Waters Acquity Set: 24112021

Sample Manager

Sample	Locations	Quantitation	Submit
(1) ANSI-48Vial2mL.Holder			
(2) ANSI-48Vial2mL.Holder			

Change the setting of sample manger ( in this case it is Water acquity SM and we are using 48 vial 2 ml holder this setting need to be put in earlier sample table too

Prepared by Amrutha N., Pallavi H.U., Dr. Ankit J., Dr. Nirpendra S.

Sample Name	Rack Position	Plate Position	Vial Position	Acquisition Method	Quantitation	Data File	Set Name	Submit Status
	1	1	1	SugarP_18082021	none	24112021\	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	Sug				
	1	1	1	Sug				
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not
	1	1	1	SugarP_18082021	none	Blank2411202	24112021	Not

Go to submit tab and submit the sample

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1	✓	22-11-2021 14:19:13	TuneSampleName	0		Acquired	s2_QOpt_BP_Pos	ManualTune	s2_BP_Pos	Defa
2	✓	22-11-2021 14:19:28	TuneSampleName	0		Acquired	s2_QOpt_InitQ1_Pos	ManualTune	s2_InitQ1_Po	Defa
3	✓	22-11-2021 14:19:35	TuneSampleName	0		Acquired	s2_QOpt_InitQ1_Pos	ManualTune	s2_InitQ1_Po	Defa
4	✓	22-11-2021 14:19:41	TuneSampleName	0		Acquired	s2_QOpt_InitQ1_Pos	ManualTune	s2_InitQ1_Po	Defa
5	✓	22-11-2021 14:19:48	TuneSampleName	0		Acquired	s2_QOpt_DP_Pos	ManualTune	s2_DP_Pos	Defa
6	✓	22-11-2021 14:20:03	TuneSampleName	0		Acquired	s2_QOpt_FinalQ1_Pos	ManualTune	s2_FinalQ1_	Defa
7	✓	22-11-2021 14:20:12	TuneSampleName	0		Acquired	s2_QOpt_InitProduct_Pos	ManualTune	s2_InitProduc	Defa
8	✓	22-11-2021 14:21:35	TuneSampleName	0		Acquired	s2_QOpt_CE_Pos	ManualTune	s2_CE_Pos	Defa
9	✓	22-11-2021 14:22:08	TuneSampleName	0		Acquired	s2_QOpt_CXP_MR0_Pos	ManualTune	s2_CXP_MR0	Defa
10	✓	22-11-2021 14:22:48	TuneSampleName	0		Acquired	s2_QOpt_CXP_MR1_Pos	ManualTune	s2_CXP_MR1	Defa
11	✓	22-11-2021 14:22:56	TuneSampleName	0		Acquired	s2_QOpt_CXP_MR2_Pos	ManualTune	s2_CXP_MR2	Defa
12	✓	22-11-2021 14:23:15	TuneSampleName	0		Acquired	s2_QOpt_FinalPrdt_Pos	ManualTune	s2_FinalPrdt_	Defa
13	⊘	22-11-2021 14:26:54	TuneSampleID	0		Terminated	testTune	ManualTune	MT20211122	API
14	⊘	22-11-2021 14:29:08	TuneSampleID	0		Terminated	testTune	ManualTune	MT20211122	API
15	⊘	22-11-2021 14:41:17	TuneSampleID	0		Terminated	testTune	ManualTune	MT20211122	API
16	⊘	22-11-2021 14:42:28	TuneSampleID	0		Terminated	testTune	ManualTune	MT20211122	API
17	⊘	22-11-2021 14:45:23	TuneSampleID	0		Terminated	testTune	ManualTune	MT20211122	API
18	⊘	22-11-2021 14:46:14	TuneSampleID	0		Terminated	testTune	ManualTune	MT20211122	API
19	✓	22-11-2021 14:53:40	TuneSampleID	0		Acquired	testTune	ManualTune	MT20211122	API
20	⊘	22-11-2021 14:58:51	TuneSampleID	0		Terminated	testTune	ManualTune	MT20211122	API
21	⊘	22-11-2021 15:02:16	3455_sample2	0		Terminated	testTune	ManualTune	Sample_2_34	Defa
22	⊘	22-11-2021 15:04:02	TuneSampleID	0		Terminated	testTune	ManualTune	MT20211122	API
23	✓	22-11-2021 15:05:54	TuneSampleID	0		Acquired	testTune	ManualTune	MT20211122	API
24	✓	22-11-2021 15:07:53	TuneSampleID	0		Acquired	testTune	ManualTune	MT20211122	API
25	✓	22-11-2021 15:11:00	3455	0		Acquired	testTune	ManualTune	Sample_2	Defa
26	⌛	24-11-2021 09:45:53	sample1	1	1	Waiting	SugarP_18082021	New Batch		202
27	⌛	24-11-2021 10:06:53	sample2	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
28	⌛	24-11-2021 10:27:53	sample3	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
29	⌛	24-11-2021 10:48:53	sample4	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
30	⌛	24-11-2021 11:09:53	sample5	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
31	⌛	24-11-2021 11:30:53	sample6	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
32	⌛	24-11-2021 11:51:53	sample7	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
33	⌛	24-11-2021 12:12:53	sample8	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
34	⌛	24-11-2021 12:33:53	sample9	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
35	⌛	24-11-2021 12:54:53	sample10	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
36	⌛	24-11-2021 13:15:53	sample11	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
37	⌛	24-11-2021 13:36:53	sample12	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202
38	⌛	24-11-2021 13:57:53						New Batch	Blank241120	202
39	⌛	24-11-2021 14:18:53						New Batch	Blank241120	202
40	⌛	24-11-2021 14:39:53	sample15	1	1	Waiting	SugarP_18082021	New Batch	Blank241120	202

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The image shows the Analyst software interface. The left-hand menu is expanded, showing various configuration and analysis options. A red arrow points from the 'MultiQuant 3.0.3' option in the menu to the text 'Open Multiquant form here and start analysing your samples'. The main area of the software is currently blank.

File Edit View Tools Window Script Help

Configure Mode Shreyas\2021\_03\_09

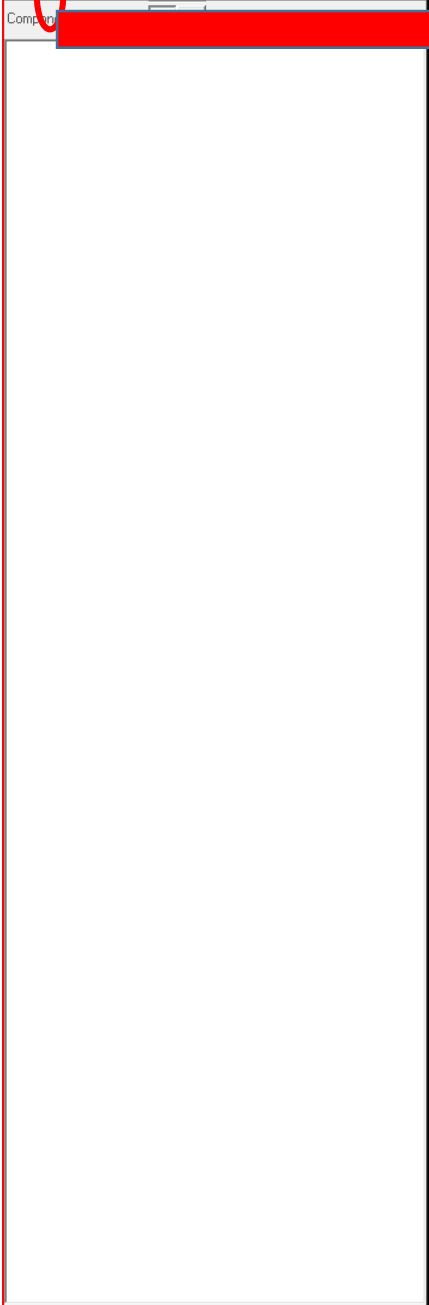
- Configure
  - Security Configuration
  - Hardware Configuration
  - Report Template Editor
- Tune and Calibrate
  - Compound Optimization
  - Instrument Optimization
  - Manual Tuning
- Acquire
  - IDA Method Wizard
  - Build Acquisition Method
  - Build Acquisition Batch
- Explore
  - Open Data File
  - Open Compound Database
- Quantitate
  - Build Quantitation Method
  - Quantitation Wizard
  - Review Results Table
- Companion Software
  - ACQUITY Console
  - ACQUITY Console Editor
  - MultiQuant 3.0.3**
  - Reporter

Open Multiquant form here and start analysing your samples

User Name: DESKTOP-STIHJ5R\sciex D:\Analyst Data

09:48 24-11-2021

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Open your raw data file ( Wiff) from here.

[Begin by creating a results table or opening an existing one.](#)

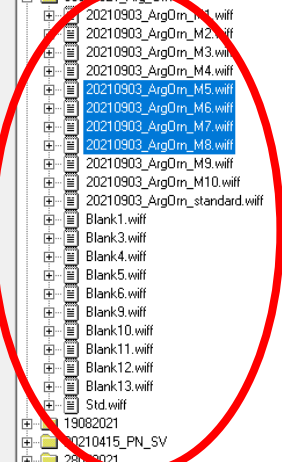


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Available

Browse...

- 13C Acetate 18hrs SD
- 13C Asp 24hrs YPD
- 13C Asp SD 12hrs
- 08022021\_Arg0rn
- 20210903\_Arg0rn\_M1.wiff
- 20210903\_Arg0rn\_M2.wiff
- 20210903\_Arg0rn\_M3.wiff
- 20210903\_Arg0rn\_M4.wiff
- 20210903\_Arg0rn\_M5.wiff
- 20210903\_Arg0rn\_M6.wiff
- 20210903\_Arg0rn\_M7.wiff
- 20210903\_Arg0rn\_M8.wiff
- 20210903\_Arg0rn\_M9.wiff
- 20210903\_Arg0rn\_M10.wiff
- 20210903\_Arg0rn\_standard.wiff
- Blank1.wiff
- Blank3.wiff
- Blank4.wiff
- Blank5.wiff
- Blank6.wiff
- Blank9.wiff
- Blank10.wiff
- Blank11.wiff
- Blank12.wiff
- Blank13.wiff
- Std.wiff
- 19082021
- 20210415\_PN\_SV
- 28082021
- A\_20210831162340
- HESC\_AA\_20210408
- HESC\_AcCoA\_20210407
- HESC\_TCA
- Ppg1 SD
- SL1\_ppg1 6hrs YPD
- Sriram
- 28082021\_Blank1.wiff
- 28082021\_Blank2.wiff
- 28082021\_Blank3.wiff
- 28082021\_Blank4.wiff
- 28082021\_Standard.wiff



Add your samples to the result table

Selected

=>

<=

Available

Browse...

- 13C Acetate 18hrs SD
- 13C Asp 24hrs YPD
- 13C Asp SD 12hrs
- 08032021\_Arg\_Drm
  - 20210903\_ArgDrm\_M1.wiif
  - 20210903\_ArgDrm\_M2.wiif
  - 20210903\_ArgDrm\_M3.wiif
  - 20210903\_ArgDrm\_M4.wiif
  - 20210903\_ArgDrm\_M9.wiif
  - 20210903\_ArgDrm\_M10.wiif
  - 20210903\_ArgDrm\_standard.wiif
  - Blank1.wiif
  - Blank3.wiif
  - Blank4.wiif
  - Blank5.wiif
  - Blank6.wiif
  - Blank9.wiif
  - Blank10.wiif
  - Blank11.wiif
  - Blank12.wiif
  - Blank13.wiif
  - Std.wiif
- 19082021
- 20210415\_PN\_SV
- 28052021
- A\_20210831162340
- HESC\_AA\_20210408
- HESC\_AcCoA\_20210407
- HESC\_TCA
- Ppg1 SD
- SL1 ppg1 6hrs YPD
- Sriram
- 28082021\_Blank1.wiif
- 28082021\_Blank2.wiif
- 28082021\_Blank3.wiif
- 28082021\_Blank4.wiif
- 28082021\_Standard.wiif

Selected

- 08032021\_Arg\_Drm
  - 20210903\_ArgDrm\_M5.wiif
    - M5
  - 20210903\_ArgDrm\_M6.wiif
    - M6
  - 20210903\_ArgDrm\_M7.wiif
    - M7
  - 20210903\_ArgDrm\_M8.wiif
    - M8

=>

=<

Select an existing quantitation method or create a new method now.

Choose Existing Method

Method Name:  Open...

Edit Method

Create New Method (MQ4)

Method Name: [Click 'New' to select method](#) New...

Use 'Automatic' Method (MQ4)

(Created on-the-fly and most useful when MRM transitions differ between samples)

Either use the earlier processing method or create new method ( automatic method ( MQ4)



Select or verify the analyte and internal standard names and masses.

Experiment: MRM (2 transitions)

Row	IS	Name	Group	IS Name	Q1/Q3
1	<input type="checkbox"/>	Arg			175.2 / 60.2
2	<input checked="" type="checkbox"/>	Om			133.0 / 70.1
3	<input type="checkbox"/>				

**All the transition selected in the MRM method will be uploaded here ,please define which is your internal control here and any grouping. Click next**

Set criteria for flagging outliers.

<input checked="" type="checkbox"/> Accuracy for Standards	<input checked="" type="checkbox"/> Accuracy for QCs
Max. Accuracy Tolerance for LLOQ (lowest Std): <input type="text" value="20"/> %	Max. Accuracy Tolerance for QC: <input type="text" value="15"/> %
Max. Accuracy Tolerance for Stds except LLOQ: <input type="text" value="15"/> %	

Ion Ratio  Calculated Concentration

Component	Lower Limit of Calculated Concentration	Upper Limit of Calculated Concentration
Arg	2	5
Om		

**Fill the Lowest limit of calculated concentration and upper limit of calculated concentrations and next**

Please select your desired units and calibration options.

Concentration Units:

Internal Calibration

Regression Parameter:

Regression Type:

Weighting Type:

**Mention about the concentration unit ( in ug/ng/pg/ppm) and regression parameter as Area not as height**

- All Components
- All Internal Standards
- Om
- All Analytes
- Arg

Name	Acquisition Date & Time	Vial Number	Acq. Method Name	IS	Component Name	Mass Info	IS Name	Component Group Name	Conc. Units	Outlier Reasons	Actual Concentration	Area	IS Area	Corrected Area	IS Correct. Area	Area Ratio	
1	M5	09-03-2021 19:52:47	7	20210903_Shreyas_Arg...	<input type="checkbox"/>	Arg	175.2 / 60.2	(No IS)		ng	Concent...	N/A	3.842e6	N/A	3.842e6	N/A	N/A
2	M5	09-03-2021 19:52:47	7	20210903_Shreyas_Arg...	<input checked="" type="checkbox"/>	Om	133.0 / 70.1	N/A		ng		1.00	3.225e5	N/A	3.225e5	N/A	N/A
3	M6	09-03-2021 20:14:37	8	20210903_Shreyas_Arg...	<input type="checkbox"/>	Arg	175.2 / 60.2	(No IS)		ng	Concent...	N/A	5.937e4	N/A	5.937e4	N/A	N/A
4	M6	09-03-2021 20:14:37	8	20210903_Shreyas_Arg...	<input checked="" type="checkbox"/>	Om	133.0 / 70.1	N/A		ng		1.00	3.143e5	N/A	3.143e5	N/A	N/A
5	M7	09-03-2021 20:36:27	9	20210903_Shreyas_Arg...	<input type="checkbox"/>	Arg	175.2 / 60.2	(No IS)		ng	Concent...	N/A	4.707e6	N/A	4.707e6	N/A	N/A
6	M7	09-03-2021 20:36:27	9	20210903_Shreyas_Arg...	<input checked="" type="checkbox"/>	Om	133.0 / 70.1	N/A		ng		1.00	2.151e5	N/A	2.151e5	N/A	N/A
7	M8	09-03-2021 20:58:19	10	20210903_Shreyas_Arg...	<input type="checkbox"/>	Arg	175.2 / 60.2	(No IS)		ng	Concent...	N/A	5.800e4	N/A	5.800e4	N/A	N/A
8	M8	09-03-2021 20:58:19	10	20210903_Shreyas_Arg...	<input checked="" type="checkbox"/>	Om	133.0 / 70.1	N/A		ng		1.00	4.239e5	N/A	4.239e5	N/A	N/A



Click here to get the peak

All Components

All Internal Standards

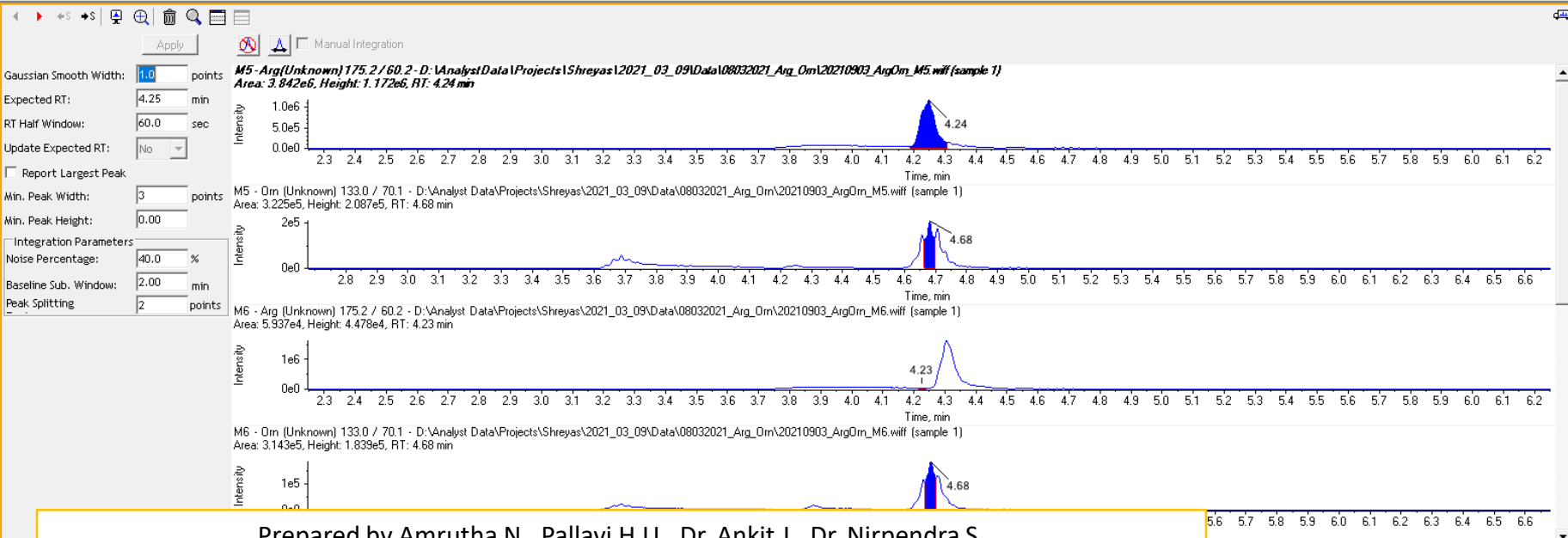
Om

All Analytes

Arg

Index	Sample Name	Acquisition Date & Time	Vial Number	Acq. Method Name	IS	Component Name	Mass Info	IS Name	Component Group Name	Conc. Units	Outlier Reasons	Actual Concentration	Area	IS Area	Corrected Area	IS Corrected Area	Area Ratio
1	M5	09-03-2021 19:52:47	7	20210903_Shreyas_Arg...	<input type="checkbox"/>	Arg	175.2 / 60.2	(No IS)		ng	Concent...	N/A	3.842e6	N/A	3.842e6	N/A	N/A
2	M5	09-03-2021 19:52:47	7	20210903_Shreyas_Arg...	<input checked="" type="checkbox"/>	Om	133.0 / 70.1	N/A		ng		1.00	3.225e5	N/A	3.225e5	N/A	N/A
3	M6	09-03-2021 20:14:37	8	20210903_Shreyas_Arg...	<input type="checkbox"/>	Arg	175.2 / 60.2	(No IS)		ng	Concent...	N/A	5.937e4	N/A	5.937e4	N/A	N/A
4	M6	09-03-2021 20:14:37	8	20210903_Shreyas_Arg...	<input checked="" type="checkbox"/>	Om	133.0 / 70.1	N/A		ng		1.00	3.143e5	N/A	3.143e5	N/A	N/A
5	M7	09-03-2021 20:36:27	9	20210903_Shreyas_Arg...	<input type="checkbox"/>	Arg	175.2 / 60.2	(No IS)		ng	Concent...	N/A	4.707e6	N/A	4.707e6	N/A	N/A
6	M7	09-03-2021 20:36:27	9	20210903_Shreyas_Arg...	<input checked="" type="checkbox"/>	Om	133.0 / 70.1	N/A		ng		1.00	2.151e5	N/A	2.151e5	N/A	N/A
7	M8	09-03-2021 20:58:19	10	20210903_Shreyas_Arg...	<input type="checkbox"/>	Arg	175.2 / 60.2	(No IS)		ng	Concent...	N/A	5.800e4	N/A	5.800e4	N/A	N/A
8	M8	09-03-2021 20:58:19	10	20210903_Shreyas_Arg...	<input checked="" type="checkbox"/>	Om	133.0 / 70.1	N/A		ng		1.00	4.239e5	N/A	4.239e5	N/A	N/A

Export your data in CSV/Excel and process further if needed. Check each peak and its marking, if needed change the Gaussian smoothing factor.



Prepared by Amrutha N., Pallavi H.U., Dr. Ankit J., Dr. Nirpendra S.