

# Quartet Data Portal User Guide for Metabolomic Quality

## Assessment Report

### 1. Preparation

QDP Address	<a href="https://chinese-quartet.org/">https://chinese-quartet.org/</a>
Input files	<p>The <b>file format (suffix)</b> should be <b>.csv</b>.</p> <p>The <b>data file</b> is the metabolite concentration result of metabolomics profiling. The required file format has samples in columns and two columns named "metabolites" and "HMDBID" including the names and HMDB IDs of metabolite compounds.</p> <p>The <b>metadata file</b> has the information of each sample in the data file. With columns named "col_names" (names of samples, identical to their names in the columns of data file), "strategy" (Targeted or Untargeted), "lab" (the name of lab), "sample" (D5, D6, F7 and M8 for Quartet samples), "rep" (the replicates for each sample) and "batch" (the name of batch).</p>

### 2. Log on to QDP

#### 2.1 Request for Quartet Metabolite RMs and QDP account

1) If you have a request for the reference materials, please go to <http://chinese-quartet.org/#/materials> to request the reference materials. The Quartet team will contact you for further confirming your information and send you a registration email.

Reference Materials

Quartet multi-omics reference materials of DNA, RNA, proteins, and metabolites were simultaneously manufactured from the same batch of cultured immortalized B-lymphoblastoid cell line of a specific family member of a Chinese Quartet family from Fudan Talzhou Cohort, including father (F7), mother (M8), and two monozygotic twin daughters (D5 and D6). The Quartet Reference Materials suite is intended for quality control and performance assessment of each omics profiling. It can measure and mitigate technical variation, enabling more accurate data integration in large cohort studies. The Quartet multi-omics reference materials are publicly available and accessible. The recipients of the Reference Materials are highly encouraged to share their data with Fudan University through the Quartet Data Portal in order for us to improve the reference datasets and to better serve the community.

Name of DNA Reference Material	Color
FDU_Quartet_DNA_D5_20171028	●
FDU_Quartet_DNA_D6_20171028	●
FDU_Quartet_DNA_F7_20171028	●

Name of RNA Reference Material	Color
FDU_Quartet_RNA_D5_20171028	●
FDU_Quartet_RNA_D6_20171028	●
FDU_Quartet_RNA_F7_20171028	●

Name of Protein Reference Material	Color
FDU_Quartet_Protein_D5_20171028	●
FDU_Quartet_Protein_D6_20171028	●
FDU_Quartet_Protein_F7_20171028	●

Name of Metabolite Reference Material	Color
FDU_Quartet_Metabolite_D5_20171028	●
FDU_Quartet_Metabolite_D6_20171028	●
FDU_Quartet_Metabolite_F7_20171028	●

2) If you do not have a request for the reference materials, please send an email to [quartet@fudan.edu.cn](mailto:quartet@fudan.edu.cn) for a QDP account.

## 2.2 Log on to QDP

Address: <http://chinese-quartet.org/>

The screenshot shows the Quartet Data Portal dashboard and login page. The dashboard includes a navigation menu, a search bar, and a 'Login' button highlighted with a red box. The main content area features the Quartet Project logo, a description of the project, and a 'Data Portal Summary' table. The login page includes a 'Account Login' section with input fields for username and password, and a 'Login' button.

**Data Portal Summary**  
Release v1.0 (October 18, 2021)

	Omics	Reference Materials	Reference Datasets
Cell Lines	6	20	16
Platforms	27	1323	2646

**Quartet**  
中华家系1号

For the Quality Control of Omics Data

[Account Login](#)

Please enter your username.

Please enter your password.

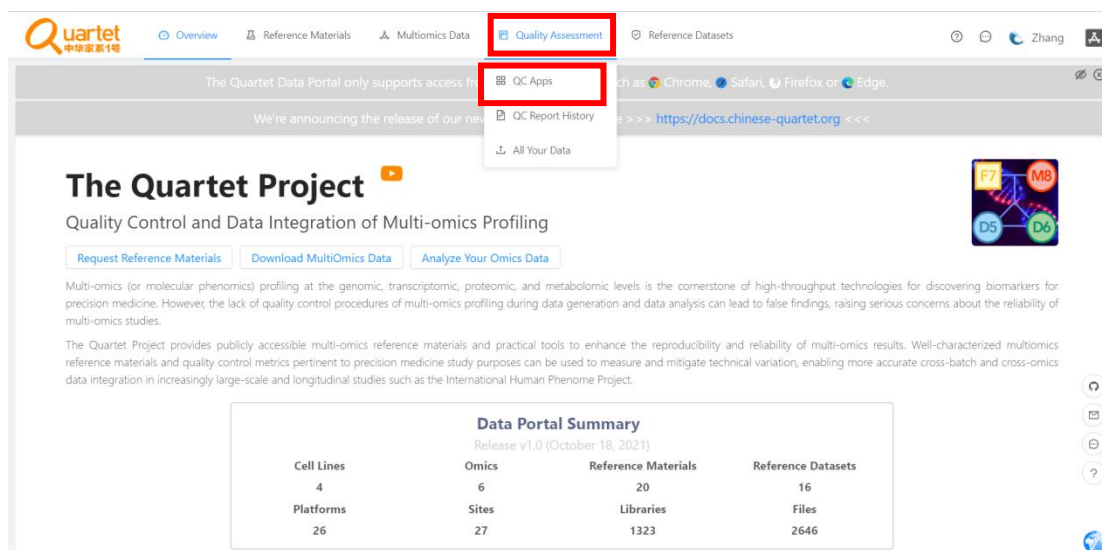
[Register](#) [Forgot Password?](#)

[Login](#)

[Data Policies](#) [Help](#) [Feedback](#)

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## 2.3 Select Quality Assessment > QC Apps

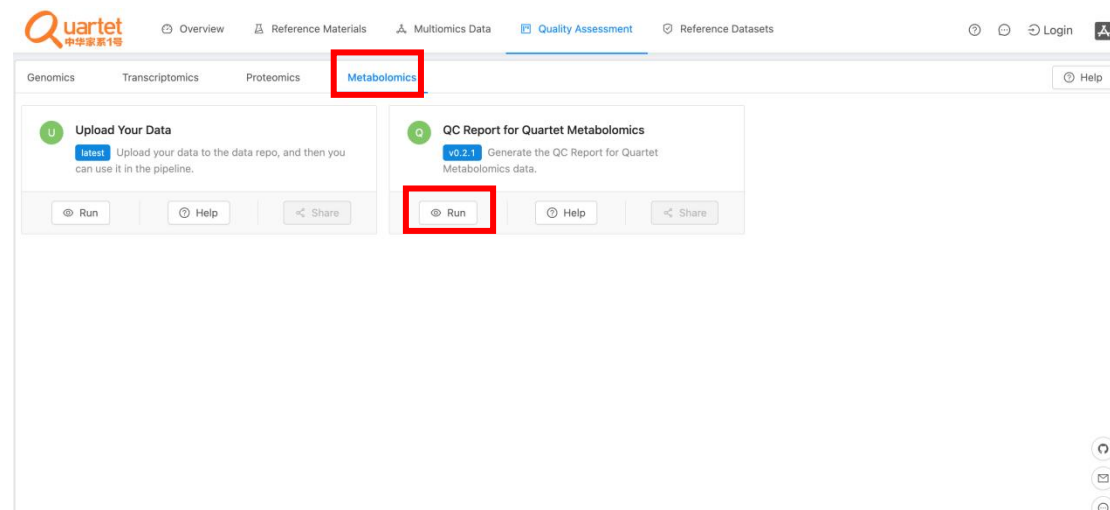


The screenshot shows the Quartet Data Portal website. The navigation menu at the top includes: Overview, Reference Materials, Multiomics Data, Quality Assessment, and Reference Datasets. The 'Quality Assessment' menu is expanded, showing 'QC Apps', 'QC Report History', and 'All Your Data'. The main content area features the title 'The Quartet Project' and the subtitle 'Quality Control and Data Integration of Multi-omics Profiling'. Below this are three buttons: 'Request Reference Materials', 'Download MultiOmics Data', and 'Analyze Your Omics Data'. A paragraph of text describes the importance of multi-omics profiling and the project's goal. A 'Data Portal Summary' table is displayed, showing the following data:

Data Portal Summary			
Release v1.0 (October 18, 2021)			
Cell Lines	Omics	Reference Materials	Reference Datasets
4	6	20	16
Platforms	Sites	Libraries	Files
26	27	1323	2646

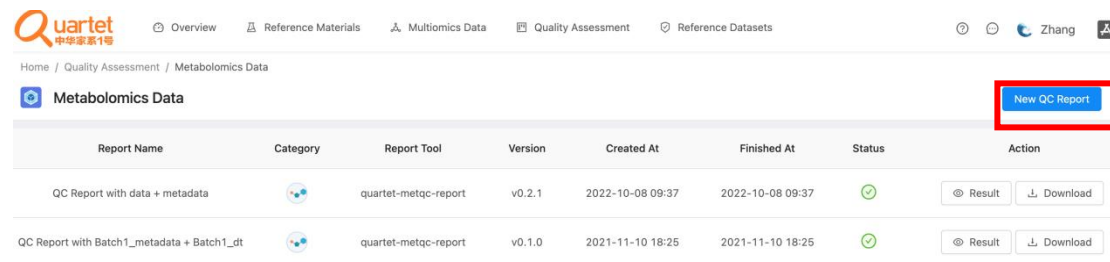
### 3. Run QC Report

#### 3.1 Select “Metabolomics” > QC Report for Quartet Metabolomics>“Run”.



The screenshot shows the Quartet web interface. The top navigation bar includes 'Overview', 'Reference Materials', 'Multiomics Data', 'Quality Assessment', and 'Reference Datasets'. The 'Metabolomics' tab is selected and highlighted with a red box. Below the navigation, there are two main cards. The left card is 'Upload Your Data' with a 'Run' button. The right card is 'QC Report for Quartet Metabolomics' with a 'Run' button circled in red. The interface also shows a 'Help' button and a 'Share' button for each card.

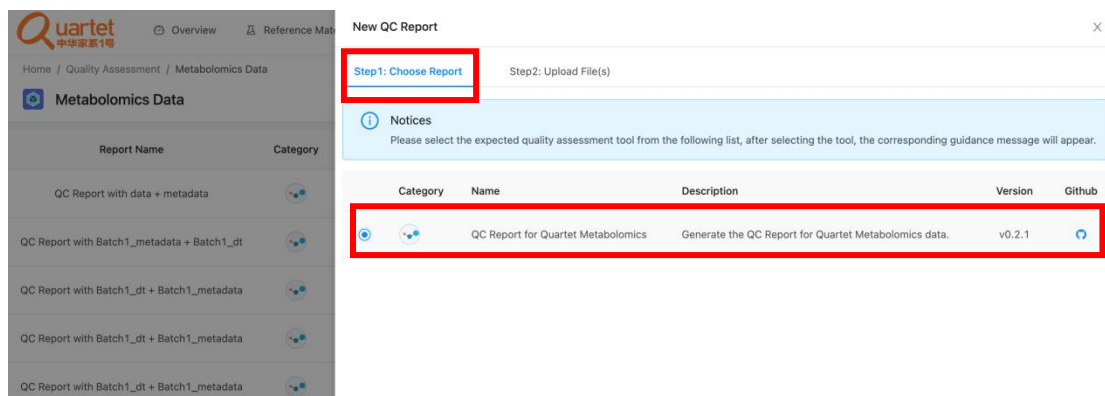
#### 3.2 Click the symbol called “New QC Report”.



The screenshot shows the Quartet web interface. The top navigation bar includes 'Overview', 'Reference Materials', 'Multiomics Data', 'Quality Assessment', and 'Reference Datasets'. The 'Metabolomics Data' section is selected. A 'New QC Report' button is highlighted with a red box. Below the button, there is a table with columns: Report Name, Category, Report Tool, Version, Created At, Finished At, Status, and Action.

Report Name	Category	Report Tool	Version	Created At	Finished At	Status	Action
QC Report with data + metadata		quartet-metqc-report	v0.2.1	2022-10-08 09:37	2022-10-08 09:37		<a href="#">Result</a> <a href="#">Download</a>
QC Report with Batch1_metadata + Batch1_dt		quartet-metqc-report	v0.1.0	2021-11-10 18:25	2021-11-10 18:25		<a href="#">Result</a> <a href="#">Download</a>

### 3.3 Select “Step1: Choose Report” > “QC Report for Quartet Metabolomics”.



Home / Quality Assessment / Metabolomics Data

Metabolomics Data

Report Name	Category
QC Report with data + metadata	
QC Report with Batch1_metadata + Batch1_dt	
QC Report with Batch1_dt + Batch1_metadata	
QC Report with Batch1_dt + Batch1_metadata	
QC Report with Batch1_dt + Batch1_metadata	

New QC Report

Step1: Choose Report Step2: Upload File(s)

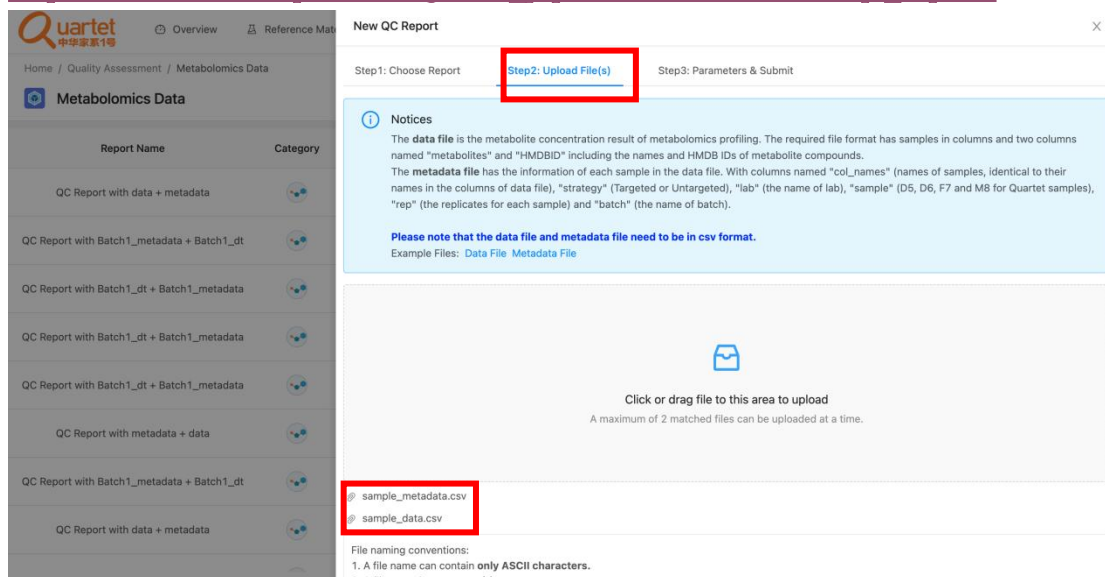
Notices  
Please select the expected quality assessment tool from the following list, after selecting the tool, the corresponding guidance message will appear.

Category	Name	Description	Version	GitHub
	QC Report for Quartet Metabolomics	Generate the QC Report for Quartet Metabolomics data.	v0.2.1	

### 3.4 Select “Step2: Upload File(s)” > “QC Report for Quartet Metabolomics”.

**Please note that the files need to be in csv format.** For details of the fixed format of the uploaded files, please refer to

[https://docs.chinese-quartet.org/data\\_pipelines/metabolomics/qc\\_report/](https://docs.chinese-quartet.org/data_pipelines/metabolomics/qc_report/)



Home / Quality Assessment / Metabolomics Data

Metabolomics Data

New QC Report

Step1: Choose Report Step2: Upload File(s) Step3: Parameters & Submit

Notices  
The **data file** is the metabolite concentration result of metabolomics profiling. The required file format has samples in columns and two columns named "metabolites" and "HMDBID" including the names and HMDB IDs of metabolite compounds.  
The **metadata file** has the information of each sample in the data file. With columns named "col\_names" (names of samples, identical to their names in the columns of data file), "strategy" (Targeted or Untargeted), "lab" (the name of lab), "sample" (D5, D6, F7 and M8 for Quartet samples), "rep" (the replicates for each sample) and "batch" (the name of batch).

**Please note that the data file and metadata file need to be in csv format.**  
Example Files: [Data File](#) [Metadata File](#)

Click or drag file to this area to upload  
A maximum of 2 matched files can be uploaded at a time.

sample\_metadata.csv  
sample\_data.csv

File naming conventions:  
1. A file name can contain **only ASCII characters**.  
2. A file name is **case-sensitive**.

3.5 After uploading the tested files, select “Step3: Parameters & Submit”. Fill in the required information and click “Submit”.

Home / Quality Assessment / Metabolomics Data

Metabolomics Data

Report Name Category

QC Report with data + metadata

QC Report with Batch1\_metadata + Batch1\_dt

QC Report with Batch1\_dt + Batch1\_metadata

QC Report with Batch1\_dt + Batch1\_metadata

QC Report with Batch1\_dt + Batch1\_metadata

QC Report with metadata + data

QC Report with Batch1\_metadata + Batch1\_dt

QC Report with data + metadata

New QC Report

Step1: Choose Report Step2: Upload File(s) Step3: Parameters & Submit

Notices

Quality Assessment of a Quartet metabolomic profiling dataset is based on built-in biological differences of the samples, consistency with the reference dataset at relative quantitation levels. The three QC metrics, including Signal-to-Noise Ratio (SNR), Correlation to reference dataset (CTR), and Root Mean Square Error (RMSE), to comprehensively assess the performance of metabolic profiles from 2 aspects: reproducibility and accuracy.

Report Name

QC Report with data + metadata

Which Report?

quartet-metqc-report

Data file

sample\_data.csv

Metadata file

sample\_metadata.csv

Description

Please input the description!

Cancel Submit

3.6 Then you can preview or download your QC report by clicking “Result” or “Download” respectively.

Home / Quality Assessment / Metabolomics Data

Metabolomics Data

New QC Report

Report Name	Category	Report Tool	Version	Created At	Finished At	Status	Action
QC Report with data + metadata		quartet-metqc-report	v0.2.1	2022-10-08 09:37	2022-10-08 09:37	✓	Result Download
QC Report with Batch1_metadata + Batch1_dt		quartet-metqc-report	v0.1.0	2021-11-10 18:25	2021-11-10 18:25	✓	Result Download