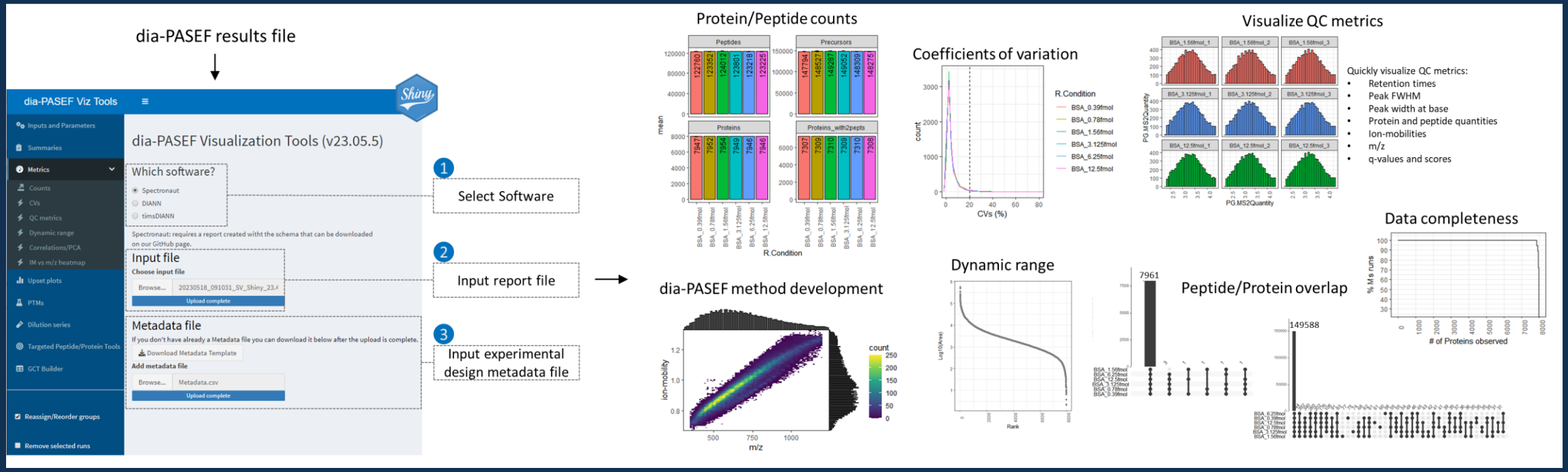
How to use the dia-PASEF Visualization Tool Shiny App



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Installation

How to install the App

- Download and unzip file:
  - Download the zipped Shiny app and save it to your local computer. Create a dedicated folder for the App. Make sure you remember the location where you saved it. And unzip the .zip file.

- Create R Project:
  - Open RStudio or any other R development environment that you prefer.
  - In RStudio, click on "File" in the top menu bar and then select "New Project". This will open a new window where you can create a new R project.
  - Choose "Existing Directory" as the project type and browse to the directory where you saved the zipped Shiny app. Click "Create Project" to create the project.
  - Make sure you have all the necessary packages installed by running install.packages(c("shiny","package2","package3")), where "package2" and "package3" represent any additional packages that the app may depend on. The file called “Install_pcks.R” lists all packages that need to be installed.

- To run the App:
  - Once the Shiny app is unzipped, you can open the “App.R" file in RStudio. Once you have installed any missing packages, you can run the Shiny app by clicking the "Run App" button in RStudio. This will start the app.

- Alternative way to run the App:
  - Another way to start the App is to run the following code in the R console: shiny::runApp(“path/to/App/folder/”)

02

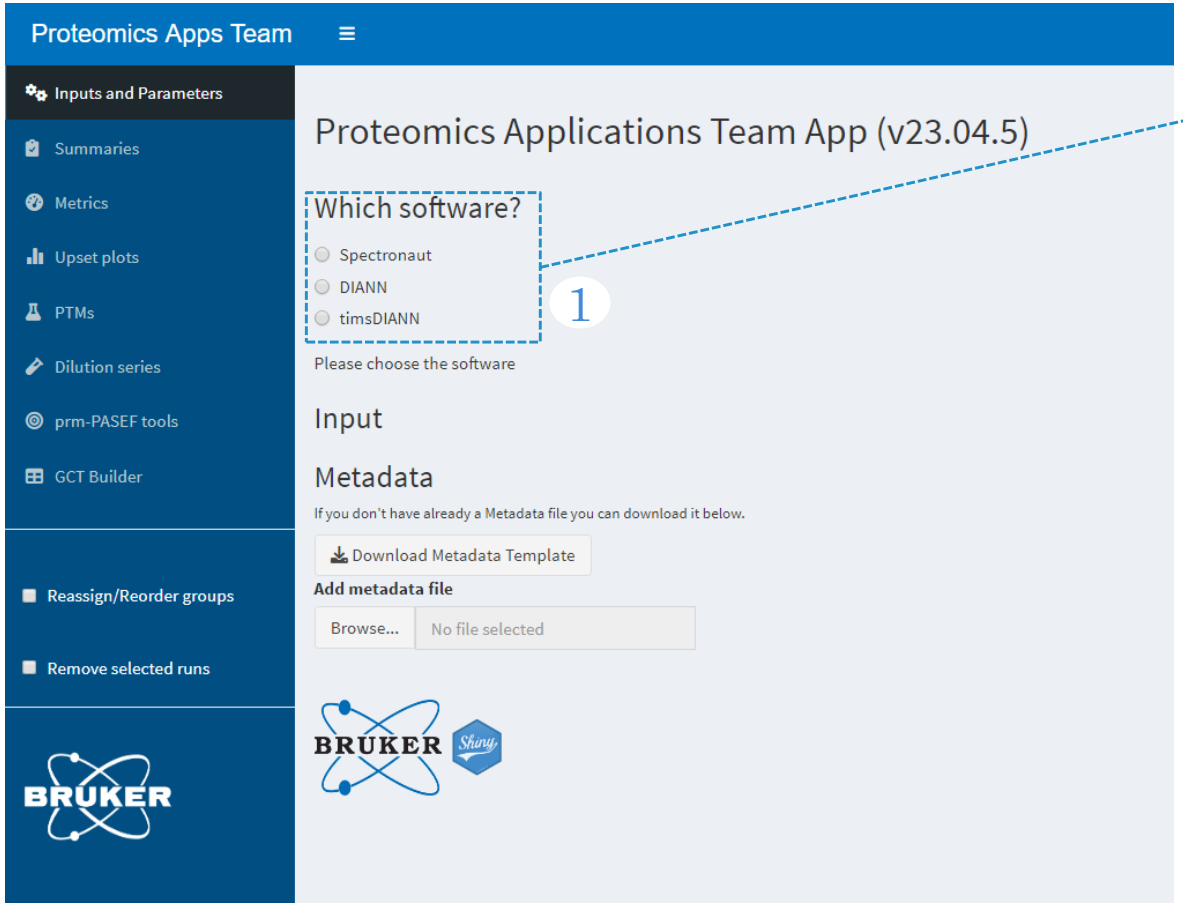
How to use the App

Inputs files

- For DIA-NN and timsDIA-NN:
  - The input file is the main report (.tsv file that does not have any suffix).
  - This file is a long format file. The app does not recognize the matrix files.
  - This file is usually the largest file

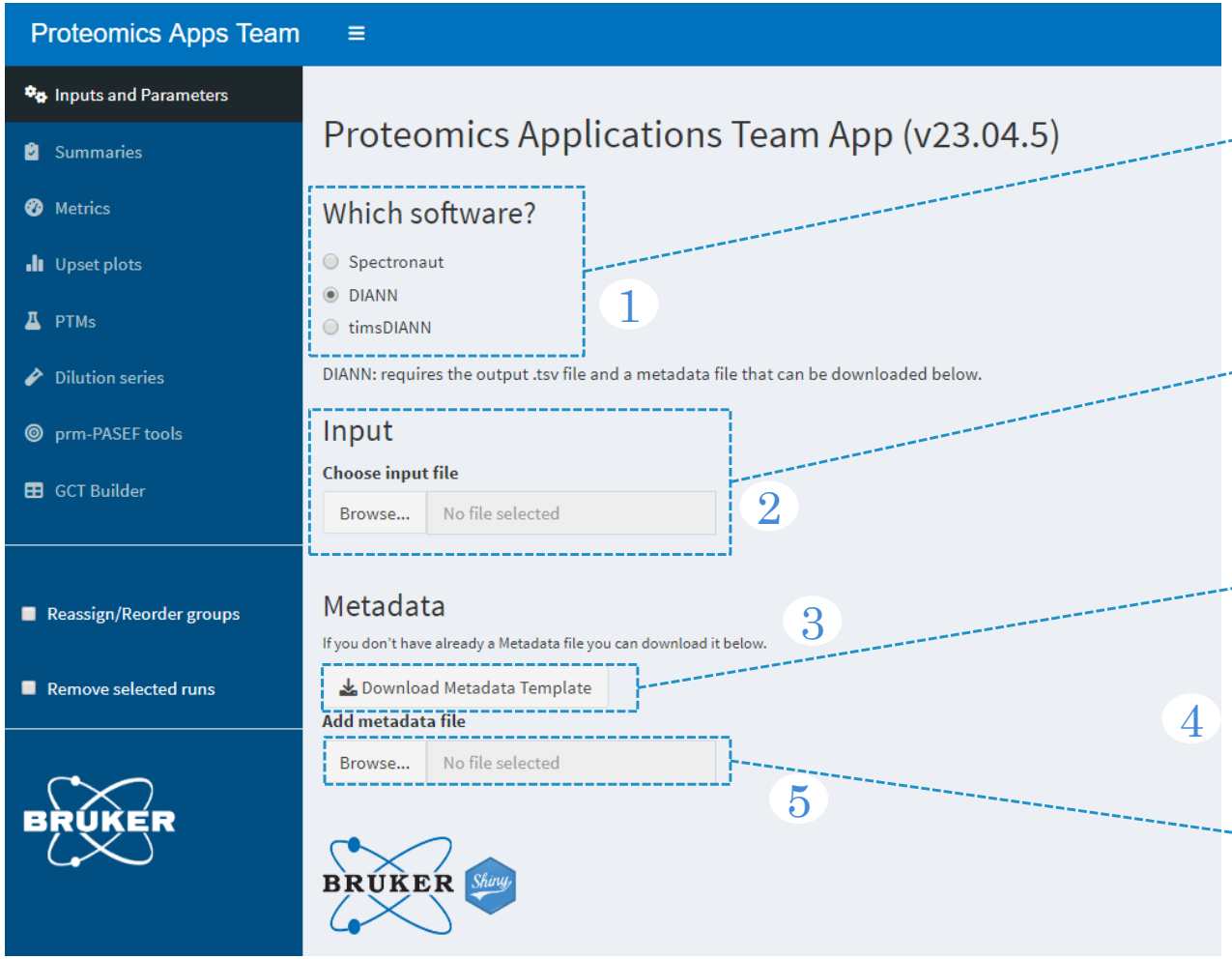
- For Spectronaut:
  - Please export the report using the template found in the folder called “Spectronaut_report_template”

Inputs and parameters



Select Software

Inputs and parameters



Select Software

Input report file

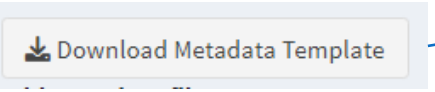
- For DIANN and TimsDIANN upload the .tsv file that contains all the information. The .tsv file with no suffixes in its name.
- For Spectronaut use the template called "SV_Shiny_23.4.06.rs"

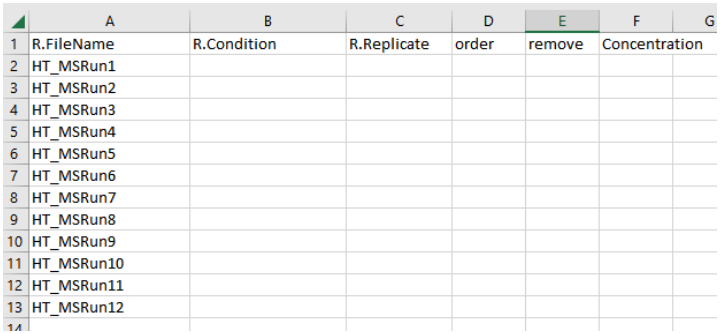
Download metadata template file

Open and complete the metadata information

Upload metadata template file

Metadata file





	A	B	C	D	E	F	G
1	R.FileName	R.Condition	R.Replicate	order	remove	Concentration	
2	HT_MSRun1						
3	HT_MSRun2						
4	HT_MSRun3						
5	HT_MSRun4						
6	HT_MSRun5						
7	HT_MSRun6						
8	HT_MSRun7						
9	HT_MSRun8						
10	HT_MSRun9						
11	HT_MSRun10						
12	HT_MSRun11						
13	HT_MSRun12						

- Download the template file
- The R.FileName column will be prefilled with the information from the quant report

	A	B	C	D	E	F
1	R.FileName	R.Condition	R.Replicate	order	remove	Concentrati
2	HT_MSRun1	K562_50ng	1	1		50
3	HT_MSRun2	K562_50ng	2	2		50
4	HT_MSRun3	K562_50ng	3	3		50
5	HT_MSRun4	K562_100ng	1	4		100
6	HT_MSRun5	K562_100ng	2	5		100
7	HT_MSRun6	K562_100ng	3	6		100
8	HT_MSRun7	K562_200ng	1	7		200
9	HT_MSRun8	K562_200ng	2	8		200
10	HT_MSRun9	K562_200ng	3	9		200
11	HT_MSRun10	K562_400ng	1	10	1	400
12	HT_MSRun11	K562_400ng	2	11	1	400
13	HT_MSRun12	K562_400ng	3	12	1	400

R.Condition:
Experimental condition

R.Replicate:
Should be unique within each condition.
No duplicates allowed within each condition

order:
Order of the plots. This sets the order for the Conditions and the MS runs for visualization.

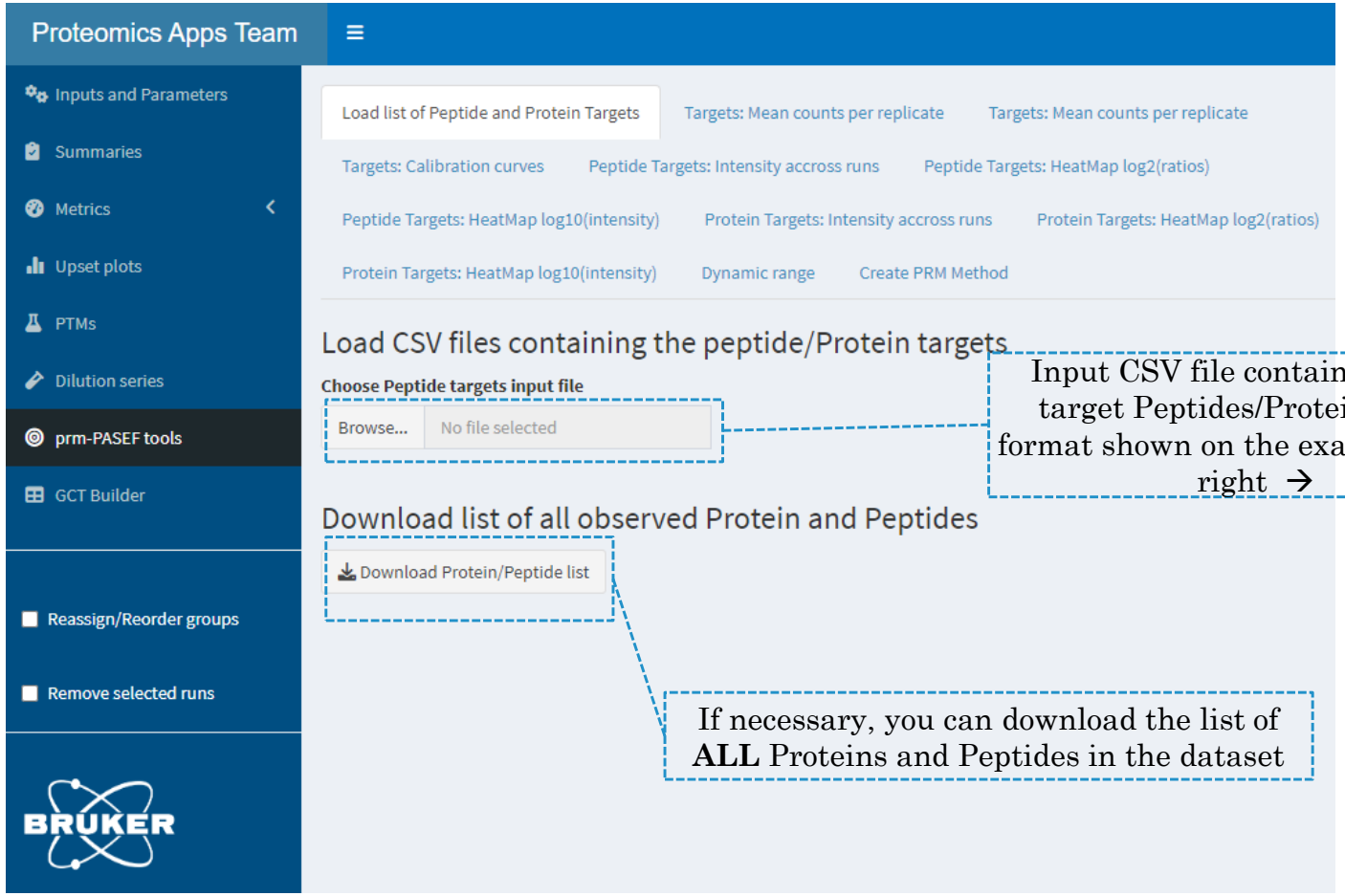
remove:
1: means you would like to remove the MS runs
Empty: means you would like to keep those MS runs

Concentration:
Should be the same value for each Condition

03

How to extract Peptide/Protein target information

Peptide/Protein target Tools



Input CSV file containing list of target Peptides/Proteins in the format shown on the example on the right →

If necessary, you can download the list of **ALL** Proteins and Peptides in the dataset

Must be a CSV File

	A	B
1	PG.ProteinGroups	EG.ModifiedPeptide
2	Protein 1	Peptide1
3	Protein 1	Peptide2
4	Protein 2	Peptide3
5	Protein 3	Peptide4
6		
7		

PG.ProteinGroups and EG.ModifiedPeptide:

- Column must be named “PG.ProteinGroups” and “EG.ModifiedPeptide”.
- The peptide sequence and protein group must exactly match the syntax of the input reports

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Disclaimer

Disclaimer

The application presented in this GitHub repository is a personal project created by Sebastian Vaca. Please note that this application is not affiliated with or supported by Bruker.

While I have made efforts to develop and test the application to the best of my abilities, I cannot guarantee its functionality, reliability, or suitability for any specific purpose. The application is provided on an "as-is" basis, and I assume no responsibility for any errors, bugs, or issues that may arise from its usage.

Furthermore, please be aware that I created this application independently and it does not fall under the scope of my responsibilities at Bruker. As a result, any inquiries, bug reports, or feature requests related to this application should not be directed to Bruker.

Please use the application at your own discretion and risk. I recommend thoroughly reviewing the code, documentation, and any associated licenses before using or modifying the application. Additionally, exercise caution when deploying the application in production environments, as it may not have undergone the same level of testing and security scrutiny as officially supported software.

If you encounter any issues or have questions about the application, I encourage you to seek assistance from the open-source community or consult the relevant documentation provided within the repository.

Thank you for your understanding and for taking note of this disclaimer.