

RGScout: A Shiny Server for Mining Resin Glycoside Information from Metabolomics (MS/MS) Data

RGScout Tutorial

Introduction

RGScout is a shiny web app in docker container as a frontend for *ResinGlycoside_Pipeline* which process metabolomics data and annotates resin glycoside like peaks. The dockerized container have everything required for executing the *ResinGlycoside_Pipeline* and finally (if everything goes perfectly well) presents output in zip compressed file. All files are important though the users may be interested to most interested in files with *.tab extension.

The ResinGlycoside Pipeline, on the other hand, is a set of scripts designed for processing LCMS data and annotating resin glycosides peaks. However, running the pipeline is not the simple and users are required to have some programming experience. Also the system requirements, software discrepancies and difficulty writing the commands are major hurdle in executing the pipeline. We, therefore, have developed RGScout which is equipped with same capabilities, but has a very user friendly environment. Users only need a working internet connection and MS data in their computer. This shiny app contains all the necessary scripts and demo files.

This tutorial will guide you through step by step process for the execution of the pipeline.

Requirements

Before proceeding, ensure that you have the following:

- Computer
- Working internet connection

Additionally, The user must obtain the following files from MS-DIAL export:

1. Peak area files (in **.txt** extensions)
2. MGF files (individual samples or aligned files in **.mgf** extensions)
3. Parameter/settings in Tab delimited files (**.tab**)

Step-by-step guide

Users may use the right panel for executing the server using their own data.

Execute

Choose MGF Files
 No file selected

Choose Peak area (TXT) Files
 No file selected

Choose Parameter File (Tab-delimited)
 No file selected

[Process Input Files](#)

[Download \(Zipped\) Processed Files](#)

[Click to Reset Session](#)

*Caution !! All the user data will be removed from the server's memory

Step 1: Provide the MGF files

Users can get this information from MS-DIAL export. The files must have a .mgf extension. Users can retrieve a sample files to know about the requisite mgf files and structure of the files.

Choose MGF Files

No file selected

Step 2: Provide the Peak Area files

Users can get this information from MS-DIAL export. The files must have a .txt extension. Users can retrieve a sample files to know about the requisite peak area files and structure of the files.

Choose Peak area (TXT) Files

No file selected

Step 3: Provide the Parameters file

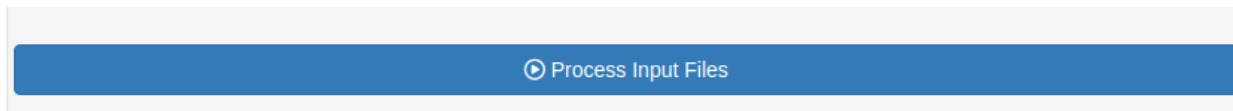
Users must provide one single Tab delimited files with .tab extension with all the parameters. Users can retrieve a sample files for the same to know about the requisite parameters files, structure of the files, or edit the prior sample information with their own settings and requisite file names and other information.

Choose Parameter File (Tab-delimited)

No file selected

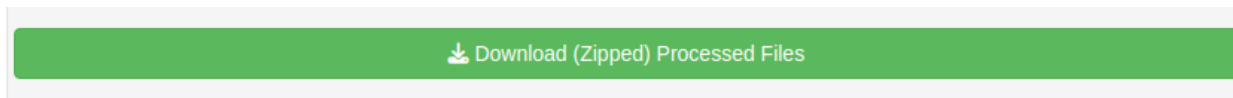
Step 4: Process the files provided

Click the processing button provide in blue colour to process the files in the required order. The details of the processing is described in the github resource (*ResinGlycoside_Pipeline*).



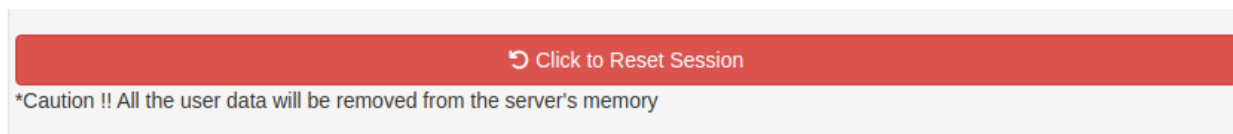
Step 5: Download the processed files

The results are provided a number of files compressed in a single zip compressed file. The number after the name of the zip files means date and time of downloading of the zip file. The number will help in citing the web-app with “retrieved on:” information. Once the data is downloaded any uploaded information or input files will be erased and the user can start another session.



Step 6: Reset the session

In case an error has occurred from user side, wrong files was input or user wants to proceed with another session, a reset button is provided. This will erase any previous information or input files and the user can restart another process.



Conclusion

RGScout is a user friendly shiny app for everyone including non-programmers to process their data to mine Resin Glycosides information from their MS/MS data. For any further questions, email Gaurav D Moghe.

Reference and Citation

For more details on RGScout and Resin Glycosides refer the following:

- Baruah VJ, and Moghe GD (2024) RGScout (Version 1) [Web-server]. <https://tools.moghelab.org/RGscout/>.
- Kruse LH, Bennett AA, Mahood EH, Lazarus E, Park SJ, Schroeder F, and Moghe GD (2022) Illuminating the lineage-specific diversification of resin glycoside acylsugars in the morning glory (Convolvulaceae) family using computational metabolomics. *Horticulture Research* 9(22), uhab079. doi: 10.1093/hr/uhab079.
- Kruse LH, Bennett AA, Baruah VJ, Irfan M, and Moghe GD (2024, under review) Extraction, annotation, and purification of resin glycosides from the morning glory family (Convolvulaceae). *Methods in Molecular Biology* doi: pending
- Any more paper for citation will be uploaded subsequently.