



Antigen Processing Likelihood Server

UPDATED: 2024/11/26, JIARUI LI

This is a guideline for Antigen Processing Likelihood Server.

The Web URL is: <https://jellyroll.cs.tulane.edu/tablex/projects/>

Please follow these steps to start.

1. Registration

First, we need to register an account, please refer to account registration guideline.

2. Quick View

After login, the dashboard will be shown.

Antigen Processing Likelihood

DASHBOARD

+ New Project

👤 Projects

🔧 Toolbox

📁 Resources

SHARE

🔗 Tool Market



New Blank Project



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It comprises 4 sections including Projects , Toolbox , Resources , and Tool Market .

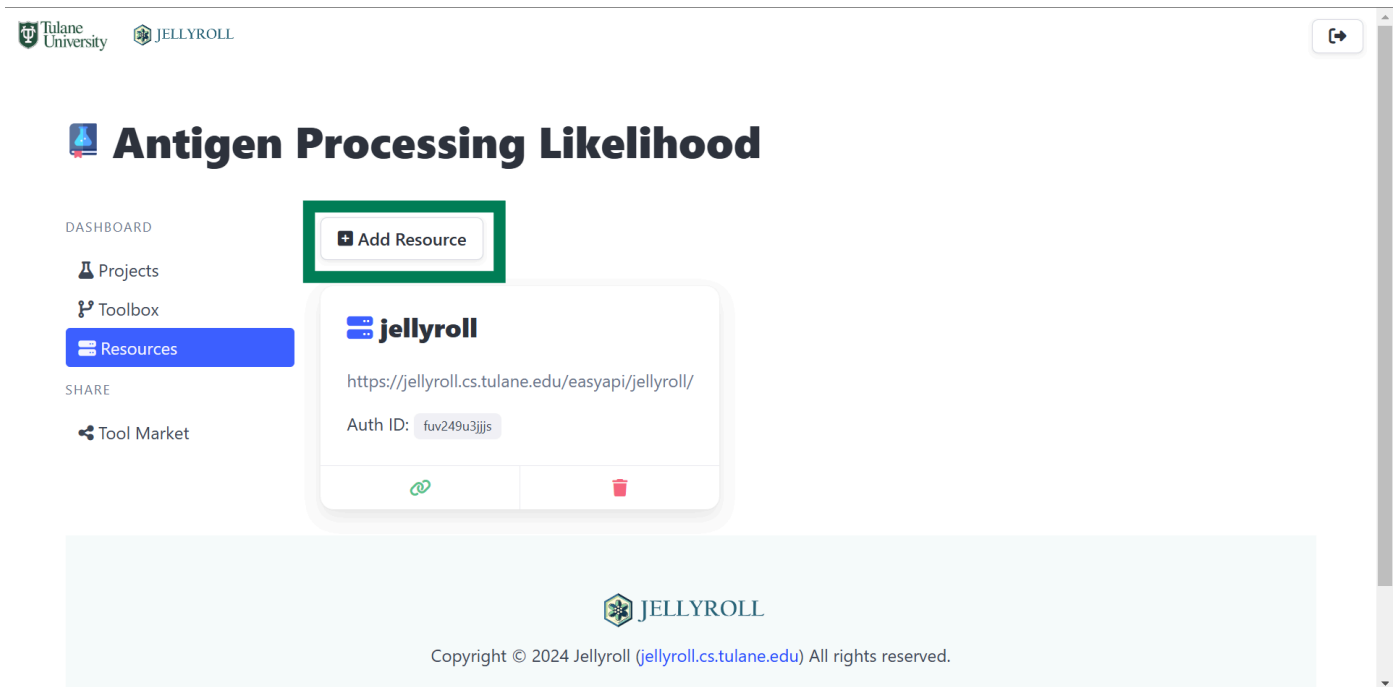
- Projects : Each running will be stored as a project and shown here as cards
- Toolbox : Each available tool will be here. And user can edit them.
- Resources : Manage all computational resources (servers).
- Tool Market : Search/Add shared tools.

3. Add Resource

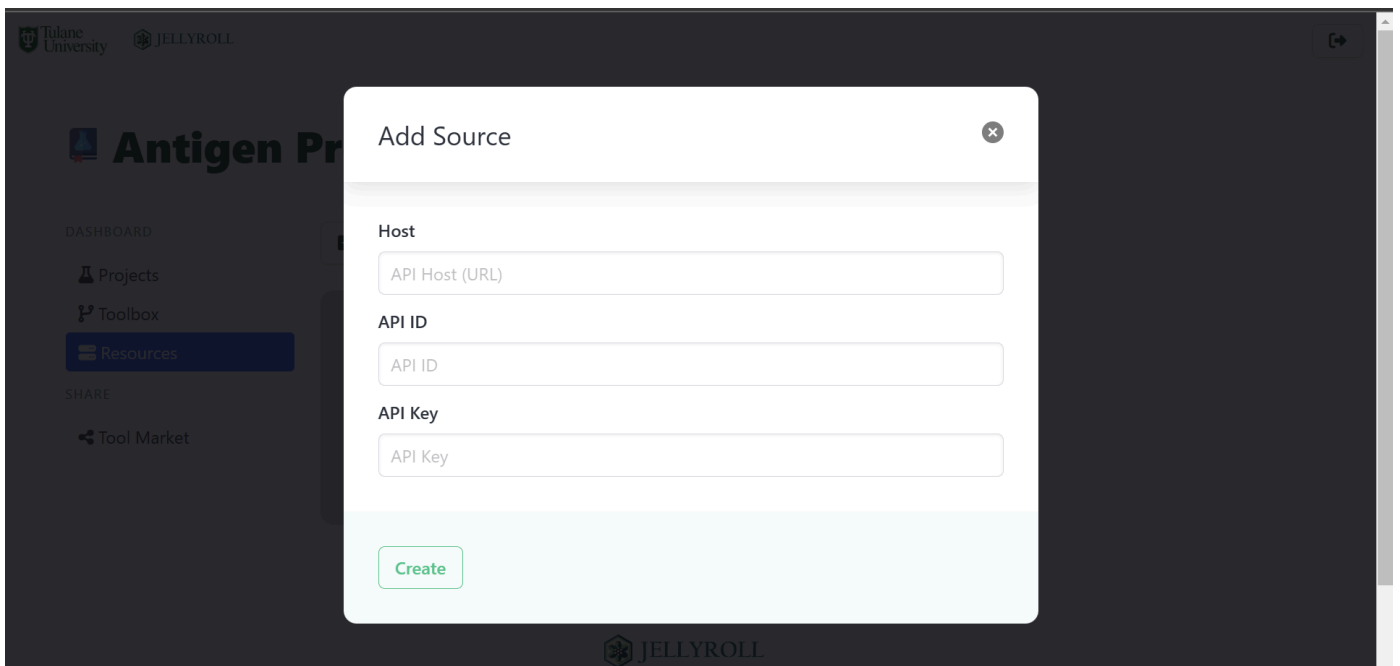
This step only needs to be finished once.

Before start, the resource required to be added first. The server connection information should be provided by service provider.

- Click Add Resource



- Fill server information and then click **create**



Then, the server should be added to your account and automatically used by each running.

Notice: There may be not only one resource/server. User could repeat this step to add more servers

4. Select Tool from Market

This step only needs to be finished once.

Go to **Tool Market** section.

Antigen Processing Likelihood

DASHBOARD

- Projects
- Toolbox
- Resources

SHARE

Tool Market

Search Tool Market

Search Tools

17 tools matched.

APL

4 blocks

It combine SASA, COREX, B-Factor, and Sequence Entropy to be APL following provided mer configuration.

Regularize Mers

1 blocks

Regularize inputed mers, which is seperated by new lines.

mmCIF to PDB

1 blocks

Transform a mmCIF protein file to a PDB file.

All shared tool is available here.

We use pure APL as an example here. (Notice: APL is only for parameter combination step. The entire APL pipeline from PDB file to APL results is provided by APL Pipeline)

First, search APL Pipeline

Antigen Processing Likelihood

DASHBOARD

- Projects
- Toolbox
- Resources

SHARE

Tool Market

Search Tool Market

APL Pipeline

3 tools matched.

APL Pipeline [AlphaFold]

13 blocks

APL Pipeline for the given AlphaFold predicted protein file (mmCIF). It will compute SASA,

APL Pipeline [RCSB]

13 blocks

APL Pipeline for given PDB ID. It will first download the PDB from RCSB. It will compute SASA,

APL Pipeline [PDB]

12 blocks

APL Pipeline for given PDB files. It will compute SASA, COREX, B-Factor, and Sequence Entropy and

There are different APL Pipeline .

- APL Pipeline [PDB] : Upload PDB files and compute APL for them.
- APL Pipeline [RCSB] : Download PDB from RCSB with provided PDB ID and compute APL for them.

- APL Pipeline [AlphaFold] : Accept AlphaFold predicted proteins (mmCIF) files and compute APL.

Click the + symbol at the bottom of the card can add this tool to your toolbox.

Let's add APL Pipeline [PDB] as example. After click + , it will automatically redirect to the copied tool edit page.

The screenshot shows the 'APL Pipeline [PDB]' tool configuration interface. At the top left, there are logos for Tulane University and JELLYROLL. A 'Dashboard' link is visible. The main title is 'APL Pipeline [PDB]'. Below the title is a table with columns for 'Order', 'Method', and various parameters. The table lists five steps: 'select_chain', 'sasa', 'bfactor', 'corex', and 'get_sequence'. Each step has associated input/output types (pdb, chain, algorithm, probe_radius, n_points, n_slices, record). To the right of the table is a 'Toolkits' sidebar with a list of tools: blast, apl_aggregate, sasa, build_mers, and combine_apl_mhc. Below the toolkits is a 'Settings' section with a 'Tool Name' input field.

Order	Method	input (required)	input (optional)	output	chain	algorithm	probe_radius	n_points	n_slices	record
0	select_chain	pdb	chain	pdb						
1	sasa	pdb				algorithm	probe_radius	n_points	n_slices	
2	bfactor	pdb								record
3	corex	pdb					probe_radius	n_points		
4	get_sequence	pdb								
5	blast									

User could edit this tool here (this only edits your copy, not the tool market one).

5. Quick Start a Tool

Then, click dashboard at the left-up corner, we could go back to dashboard.

Antigen Processing Likelihood

DASHBOARD

👤 Projects

🔧 **Toolbox**

📖 Resources

SHARE

🔗 Tool Market

+ New Tool

🔧 APL

4 blocks

It combine SASA, COREX, B-Factor, and Sequence Entropy to be APL following provided mer configuration.



🔧 APL-MHC Pipeline [AlphaFold]

16 blocks

APL-MHC Pipeline for given AlphaFold predicted protein file (mmCIF). It will compute SASA, COREX, B-Factor, and Sequence Entropy and finally combine them to be APL. Then, it uses IEDB to compute MHC-II. Finally, combined with APL.

🔧 Regularize Mers

1 blocks

Regularize inputed mers, which is seperated by new lines.



Then, click the green triangle of the selected tool, could start quick-start program, which is a guided running mode.

↔ Dashboard

🚚 Quick Start

START

🚚 **Introduction**

⚙️ Project Setting

🚚 Quick Start

APL-MHC Pipeline [PDB]

Notice

This is quick start of this tool. Under this mode, it is easier to run a tool on your data with a step-by-step guideline.

APL-MHC Pipeline for given PDB files. It will compute SASA, COREX, B-Factor, and Sequence Entropy and finally combine them to be APL. Then, it uses IEDB to compute MHC-II. Finally, combined with APL.


continue →

Click continue , user could setup the name and description for this running, or leave it as default.

[↩ Dashboard](#)

Quick Start

START

 Introduction

 Project Setting

Project Settings

APL-MHC Pipeline [PDB]

Setup the information for this running

Project Name

APL-MHC Pipeline [PDB]

Project Description

APL-MHC Pipeline for given PDB files. It will compute SASA, COREX, B-Factor, and Sequence Entropy and finally combine them to be APL. Then, it uses IEDB to compute MHC-II. Finally, combined with APL.


Then, user could upload the PDB files and parameter tables.

- Click Upload Files

[↩ Dashboard](#)

Quick Start

START

 Introduction


 Project Setting


 Data & Parameters

Data & Parameters

APL-MHC Pipeline [PDB]

These are the parameters and inputs for the computation. Provide at least one row of data to continue. The required data must be provided.

 Manually Add

 Upload Files

id

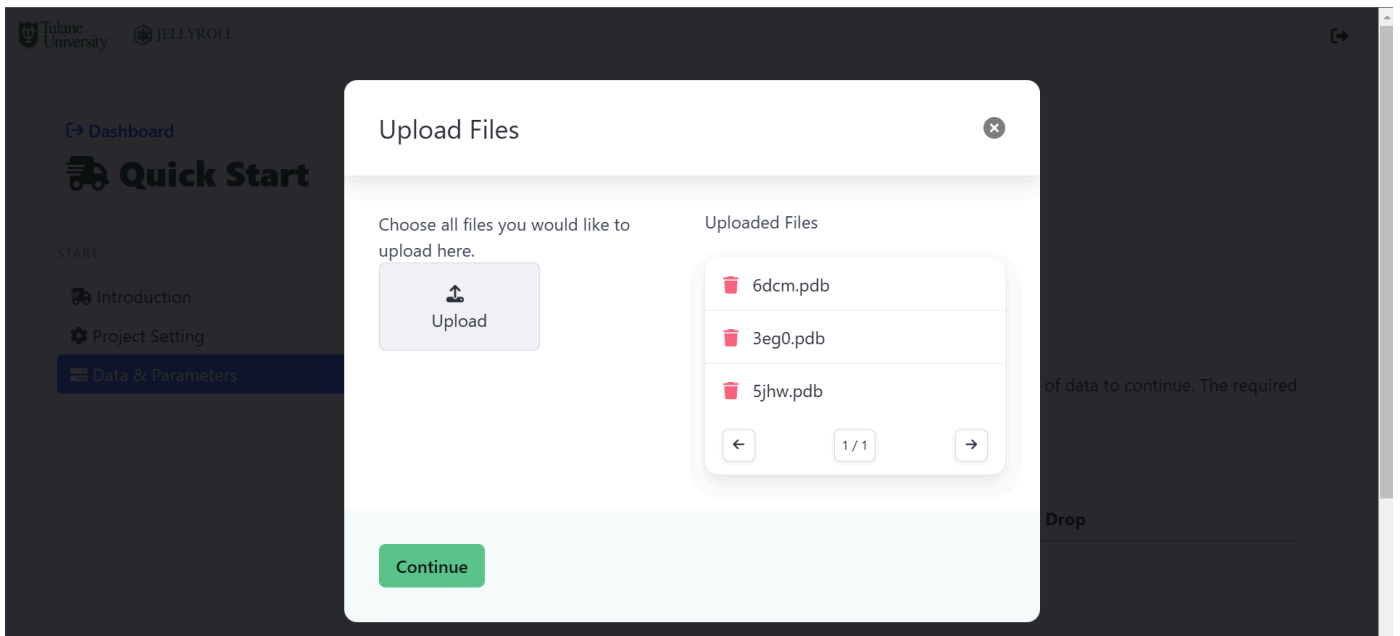
pdb

Edit

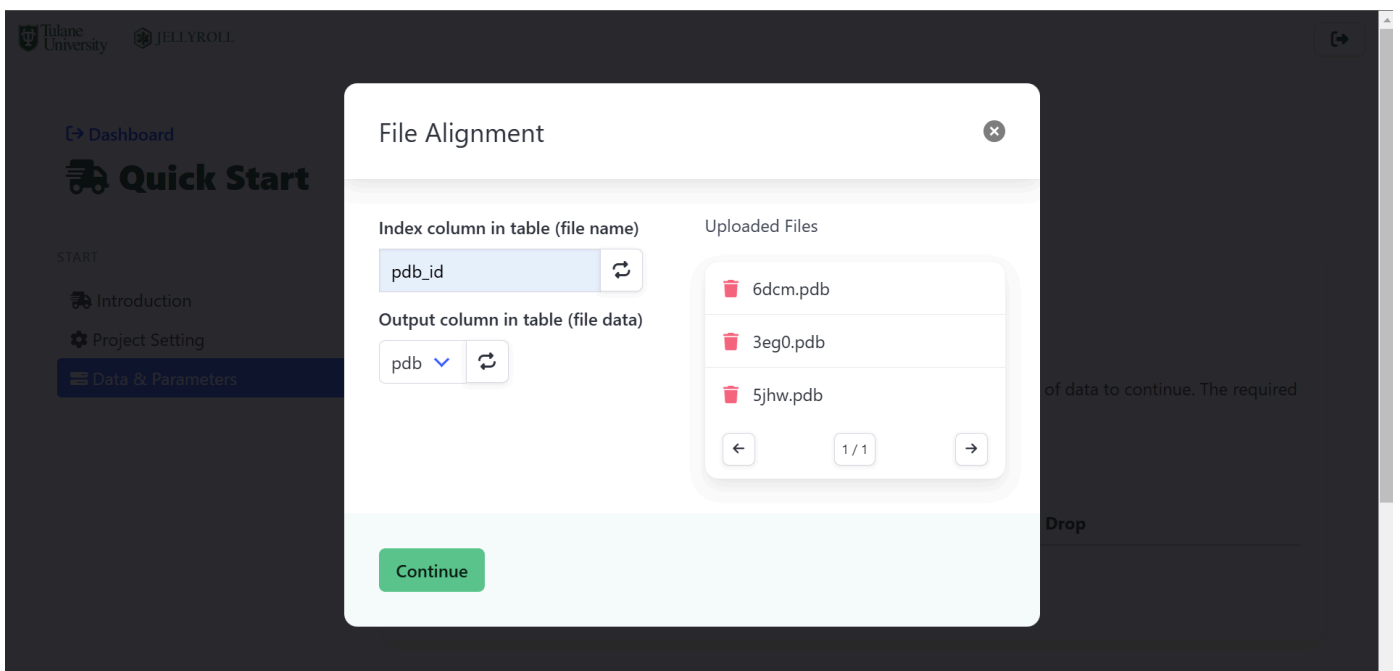
Drop

incomplete table 

- Upload PDB files. (User can add file multiple times)



- Select output column. (file name should go pdb_id column and file data should go to pdb column. Click the button next to the input box can switch to input mode.) The input should following the screenshot.



The next steps for data upload is optional, you could directly click `continue` to next step here.

Optional Steps for Paramter Customization

This section also allows to upload a CSV file with a column called `pdb_id` to customize paramter or add comment.

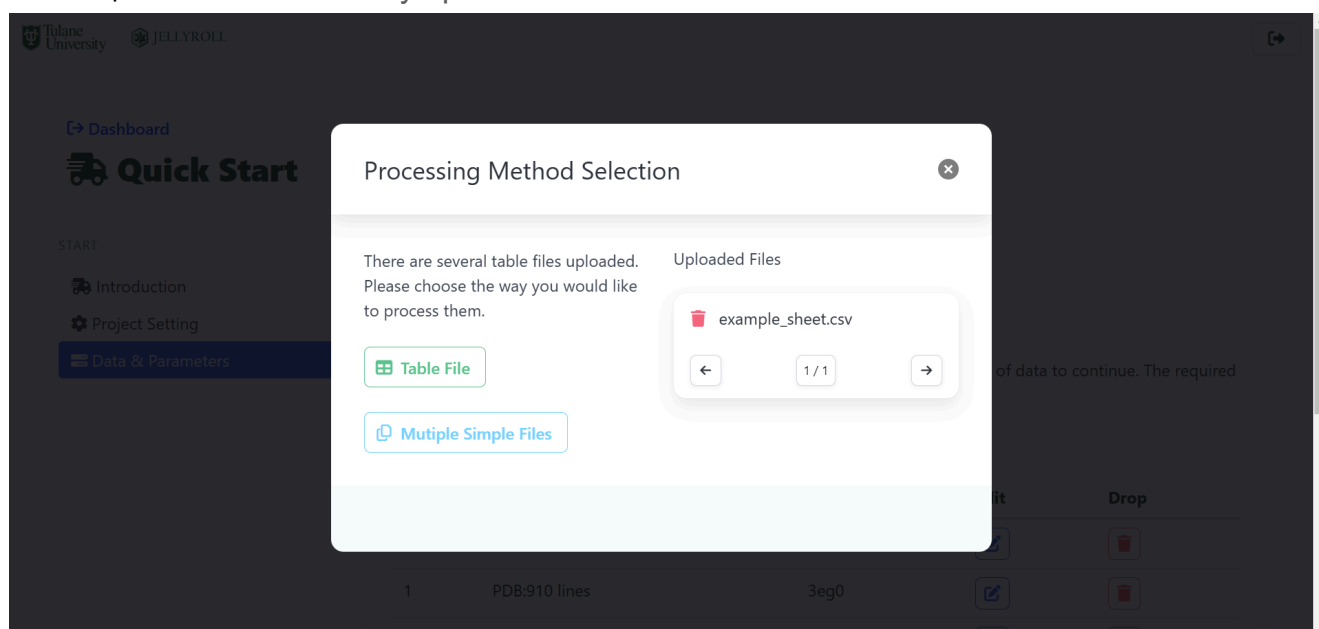
This is an example CSV

antigen,pdb_id,comment,sconf_weight
Plasminogen,6dcm,need experiment,0.5
GDF 11,5jhw,just test,
ABL1,3eg0,,0.5

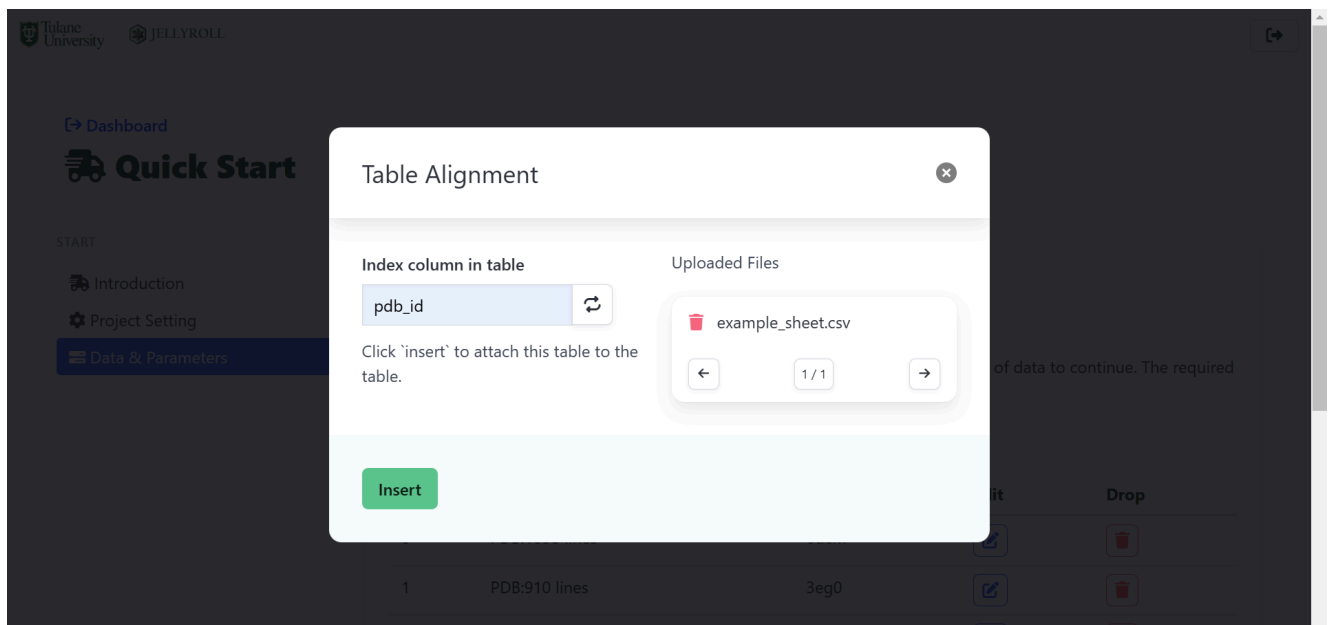
antigen	pdb_id	comment	sconf_weight
Plasminogen	6dcm	need experiment	0.5
GDF 11	5jhw	just test	
ABL1	3eg0		0.75

Each row will be matched to the PDB file row with the same pdb_id.

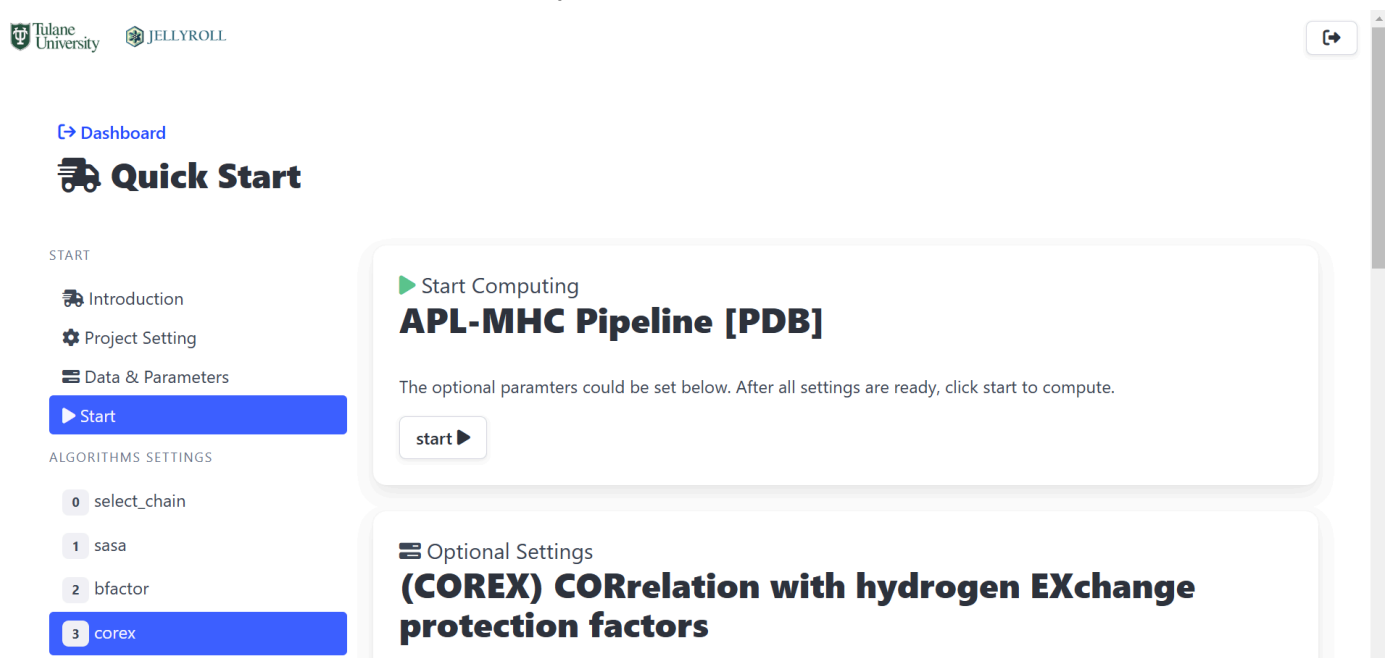
- Click **upload files** and only upload this CSV file.



- Choose **Table File** and input index column as **pdb_id**



- Click `start` to start or customize other paramter then click `start` .



6. View Result & Download

Then, it will automatically redirect to the project page.

Dashboard

APL-MHC Pipeline [PDB]

12-16-2024 07:59:38

Table

Settings

Data Table

Upload Download Add Row Drop Row Refresh

working

	pdb	pdb_id	antigen	comment	sconf_weight
1	PDB:713 lines	6dcm	Plasminogen	need experi...	0.5
2	PDB:444 lines	3eg0	ABL1		0.5
3	PDB:13467 li...	5jhw	GDF 11	just test	

Toolbox

+

APL-MHC Pipeline [PDB]

Jobs

🌙

APL-MHC Pipeline [PDB]

🏃 Get Protein Sequence

12-16-2024 08:14:59

←

1 / 1

→

The Jobs section will show current running project and its progress/status.

User could close brower/computer and go back later. No need to wait until it is finished.

Visual Result Unit

Click the cell of the table could visualize/edit the cell.

Upload Download Add Row Drop Row Refresh

ready

	apl_aggreg...	mers	regular_mers	peptide_lik...	apl_table	mhc	apl_mhc_co...	aplmhc_table
1	Residue Leve...	Protein Sequ...	Protein Sequ...	Peptide Anti...	Aggregated ...	IEDB MHCII ...	Combined A...	Aggregated ...
2	Residue Leve...	Protein Sequ...	Protein Sequ...	Peptide Anti...	Aggregated ...	IEDB MHCII ...	Combined A...	Aggregated ...
3	Residue Leve...	Protein Sequ...	Protein Sequ...	Peptide Anti...	Aggregated ...	IEDB MHCII ...	Combined A...	Aggregated ...

Update

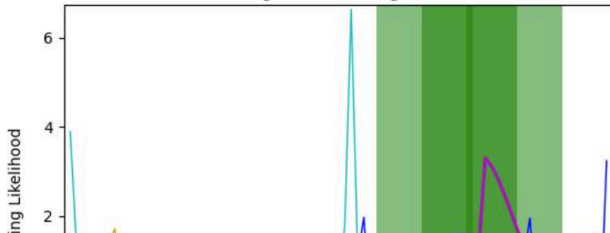
Upload

🔗 A

row: 1

column: apl_table

Plasminogen Processing Likelihood



12-16-2024 08:14:59

←

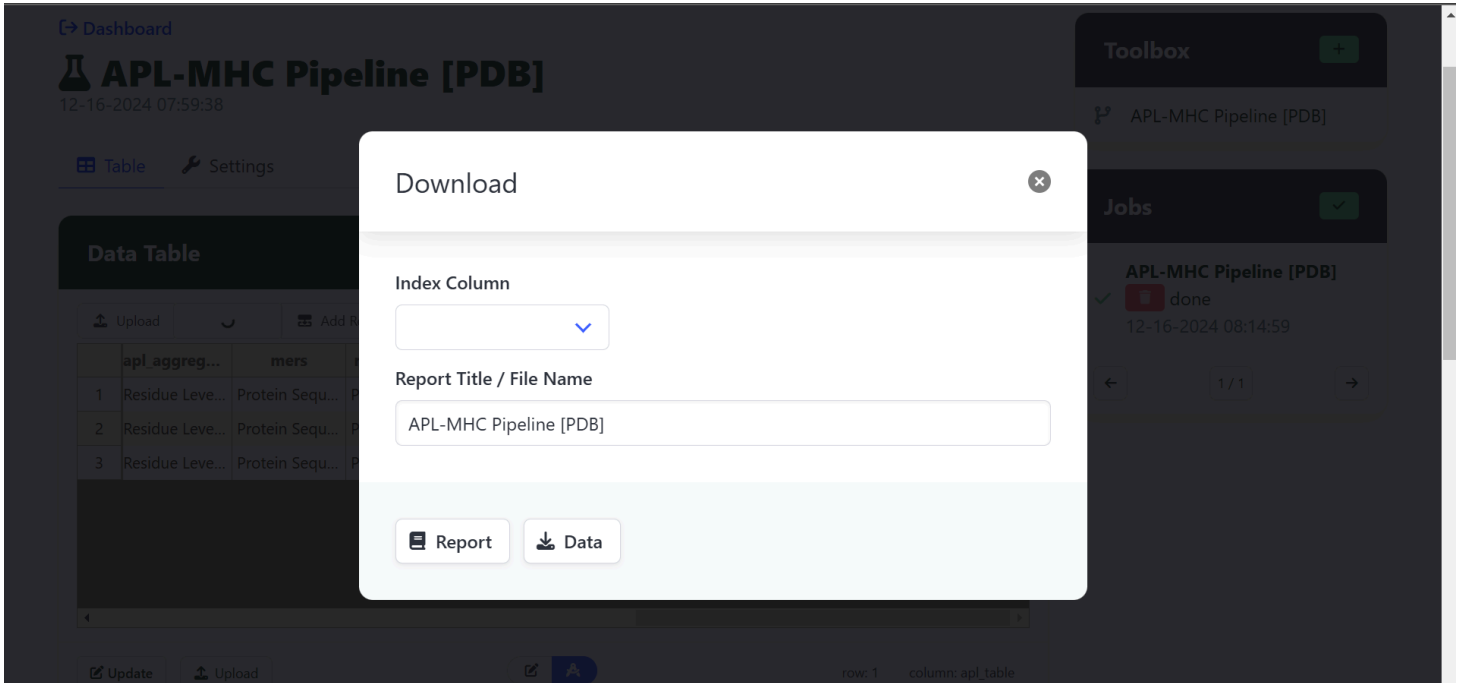
1 / 1

→

Click the switch button could switch between visulization and editor.

Download

Click download button can start to download the result.



Leave Index Column blank, it will use row number as each line name. Or user could select a column as name (e.g. antigen)

- Click Report will generate a HTML report for entire project, which could be viewed by browser and print as PDF.
- Click Data will download a ZIP file contains all data.