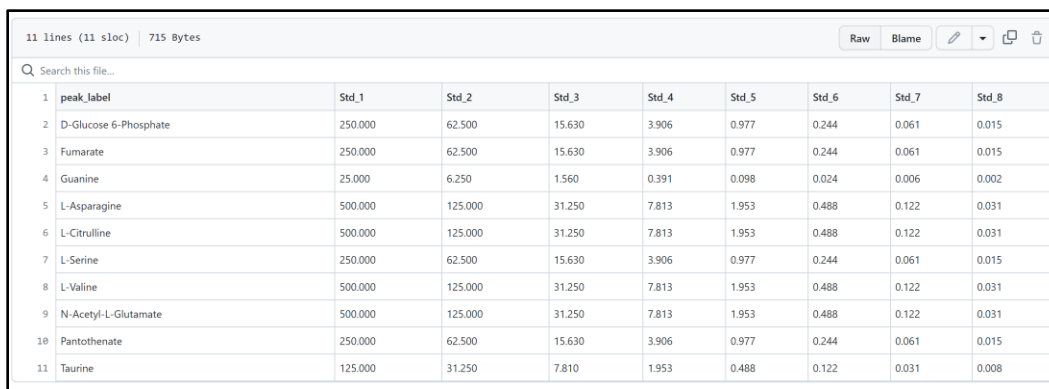


## SCALiR Tutorial

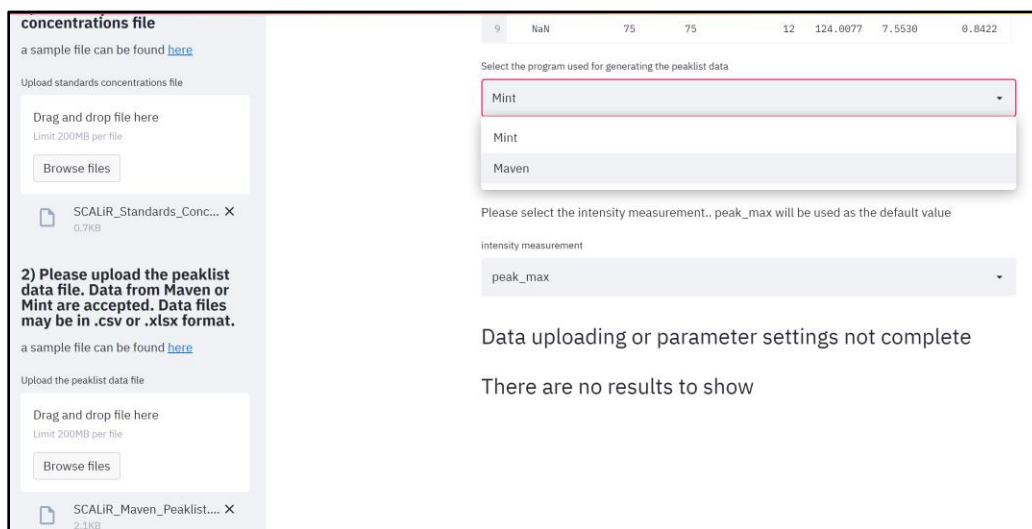
This quick (~5-10 minute) tutorial helps users understand different features of SCALiR and how to visualize and customize data generated by the app. Instructions are also available on the main page of the app.

**Step 1.** Create a new folder on your device to store the sample data upload files. Open the SCALiR web application and on the left-hand side of the screen, click on the link to the sample files. Click on the file labeled “SCALiR\_Standards\_Concentrations File”. Select the button “Raw” and then right-click to show the pop-up menu and “Save as...” to save in your folder (it should save in CSV format). Repeat this step for the three peaklist data files (two for Mint data and one for Maven data).



1	peak_label	Std_1	Std_2	Std_3	Std_4	Std_5	Std_6	Std_7	Std_8
2	D-Glucose 6-Phosphate	250.000	62.500	15.630	3.906	0.977	0.244	0.061	0.015
3	Fumarate	250.000	62.500	15.630	3.906	0.977	0.244	0.061	0.015
4	Guanine	25.000	6.250	1.560	0.391	0.098	0.024	0.006	0.002
5	L-Asparagine	500.000	125.000	31.250	7.813	1.953	0.488	0.122	0.031
6	L-Citrulline	500.000	125.000	31.250	7.813	1.953	0.488	0.122	0.031
7	L-Serine	250.000	62.500	15.630	3.906	0.977	0.244	0.061	0.015
8	L-Valine	500.000	125.000	31.250	7.813	1.953	0.488	0.122	0.031
9	N-Acetyl-L-Glutamate	500.000	125.000	31.250	7.813	1.953	0.488	0.122	0.031
10	Pantothenate	250.000	62.500	15.630	3.906	0.977	0.244	0.061	0.015
11	Taurine	125.000	31.250	7.810	1.953	0.488	0.122	0.031	0.008

**Step 2.** On the web application, upload the standards concentration file and the “SCALiR\_Maven\_Peaklist” file. The data will now pop up on the screen. Scroll down and select “Maven” in the program selection menu. The default option for slope fitting is “Fixed fit” and you should see the standard curve parameters and concentration datafiles. You can click on the highlighted links to download these files.



**concentrations file**  
a sample file can be found [here](#)

Upload standards concentrations file

Drag and drop file here  
Limit 200MB per file

Browse files

SCALiR\_Standards\_Conc... X  
0.7KB

**2) Please upload the peaklist data file. Data from Maven or Mint are accepted. Data files may be in .csv or .xlsx format.**  
a sample file can be found [here](#)

Upload the peaklist data file

Drag and drop file here  
Limit 200MB per file

Browse files

SCALiR\_Maven\_Peaklist.... X  
2.1KB

9 NaN 75 75 12 124.0877 7.5538 0.8422

Select the program used for generating the peaklist data

Mint

Mint

Maven

Please select the intensity measurement.. peak\_max will be used as the default value

intensity measurement

peak\_max

Data uploading or parameter settings not complete

There are no results to show

**Step 3.** Scroll down to the bottom of the page. The app is displaying the default metabolite. Click on the compound menu and select “Fumarate”. You can now change the axis labels on the displayed graph.

select the compound D-Glucose 6-Phosphate will be used by default

Fumarate

Fumarate

	peak_label	value	pred_conc	Concentration	Corr_Concentration
71	Fumarate	1,773.9900	0.0210	0.0150	0.0150
61	Fumarate	4,783.9800	0.0566	0.0610	0.0610
51	Fumarate	16,131.9700	0.1908	0.2440	0.2440
41	Fumarate	77,585.8400	0.9178	0.9770	0.9770
31	Fumarate	364,245.5000	4.3089	3.9060	3.9060
21	Fumarate	1,424,549.1200	16.8519	15.6300	15.6300
11	Fumarate	5,775,193.5000	68.3182	62.5000	62.5000
1	Fumarate	17045386	201.6401	250	250

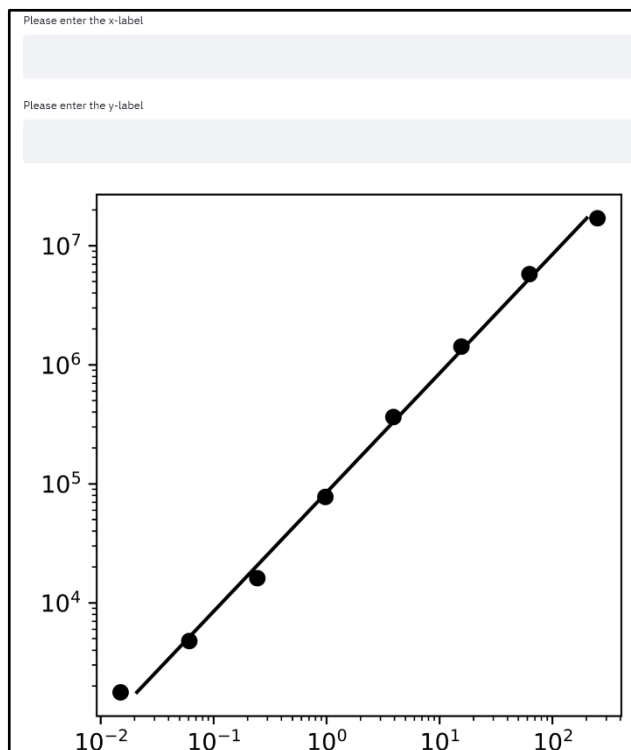
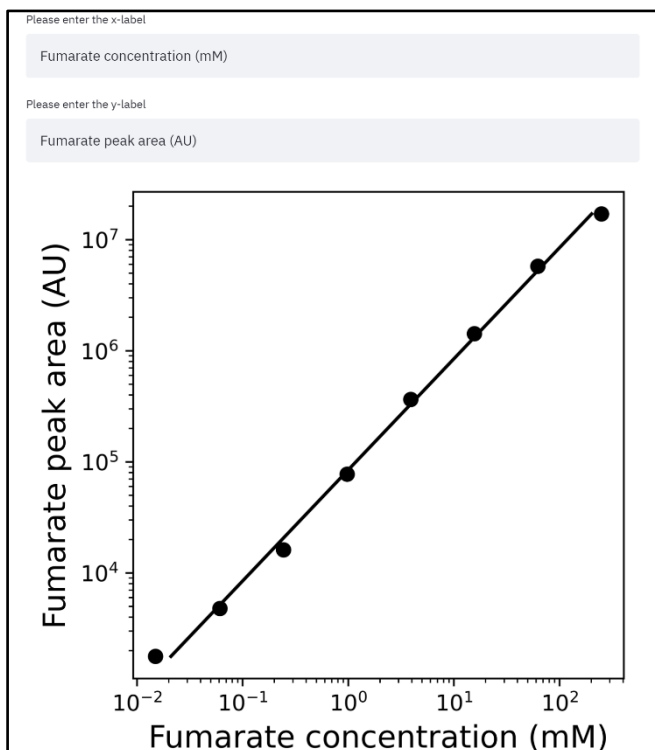
Please enter the x-label

Fumarate concentration (μM)

Please enter the y-label

Fumarate intensity (AU)

**Step 4.** Change the x-axis label to “Fumarate concentration (mM)” and click enter. Then change the y-axis label to “Fumarate peak area (AU)” and click enter. If you would like to leave the axis labels blank, delete all text in the box and click enter. To download the plot, right-click and select “Save as.”.



**Step 5.** Refresh the browser. Upload the sample standards concentrations and the “MINT Peaklist\_Full Results” files. The default program and table type are Mint and full results, so you do not need to change those but can select “peak\_area” under the intensity measurement menu. Also, select “Interval fit” under the line of best fit menu. Change the slider bar to 0.90 – 1.10 from the recommended interval of 0.85 to 1.15. SCALiR will re-run the algorithm and your new results will pop up below as before so you can download the data files as well as standard curve visualizations.

Select the program used for generating the peaklist data  

Mint

Indicate the type of table used, see Mint documentation for details  

full results

Please select the intensity measurement.. peak\_max will be used as the default value  
intensity measurement  

peak\_area

Select the flexibility for your line of best fit  

Interval fit – bounds for slope values can be defined. The interval 0.85-1.15 is recommen...

interval  
Select a range of values  

0.90

1.10

0.00

2.00

0

0.9000

1

1.1000

The standard curves have been fitted. You can download the parameters of the standard curves.

	peak_label	log_scale_slope	log_scale_intercept	N_points
0	D-Glucose 6-Phosphate	0.954676291747821	-13.009818905382717	8
1	Fumarate	0.9690645601063017	-14.564577889091881	8
2	Guanine	1.1	-18.56826969713626	6
3	L-Asparagine	0.9	-10.792403612419173	8