SCryPTA - Small Angle Scattering Crystallographic Peak Treatment and Analysis - Instructions manual

1- Introduction

The program is intended to analyze SAXS data of crystal structures of self-assembly systems. It can be accessed via the link **www.if.usp.br/scrypta**. The current supported crystal structures are:

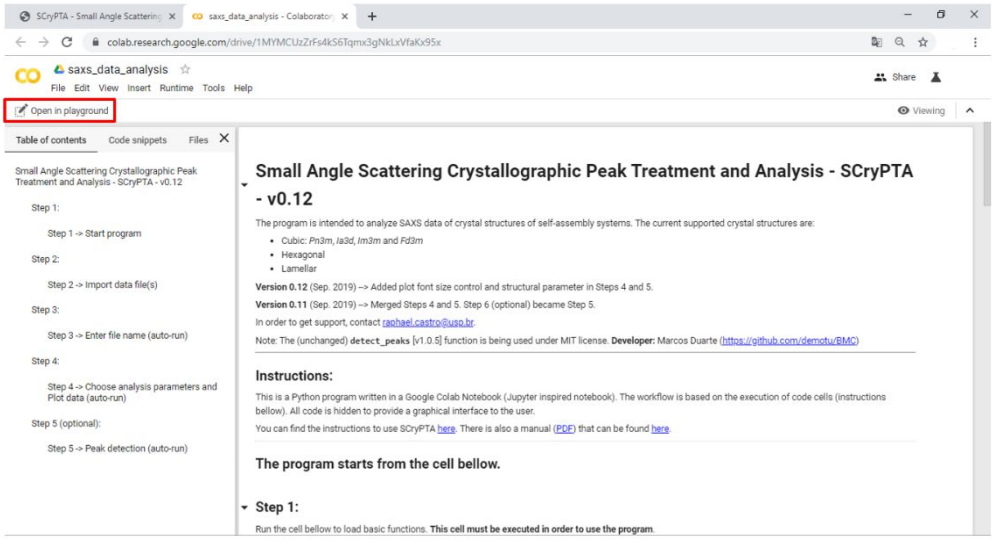
Cubic: Pn3m, Ia3d, Im3m and Fd3m;

Hexagonal;

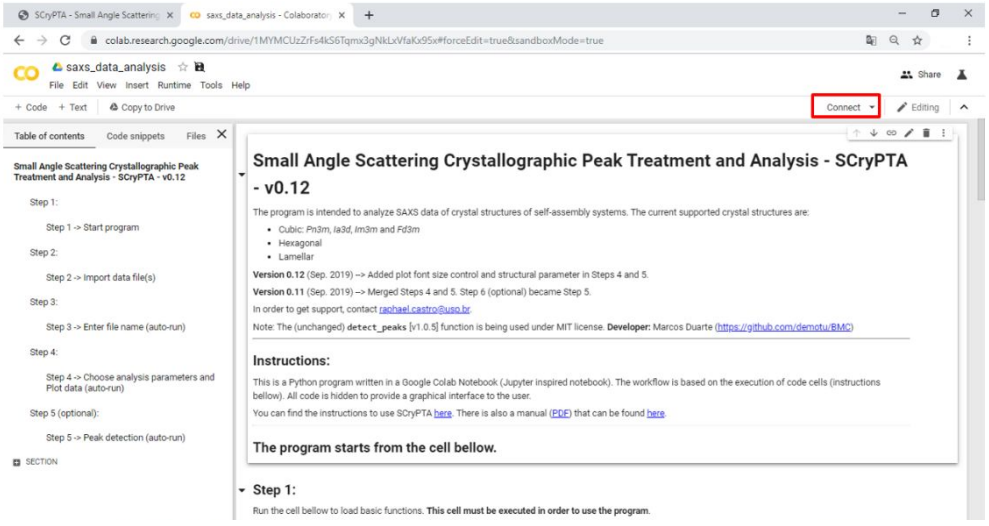
Lamellar.

Note: The (unchanged) detect_peaks [v1.0.5] function is being used under MIT license. Developer: Marcos Duarte (https://github.com/demotu/BMC).

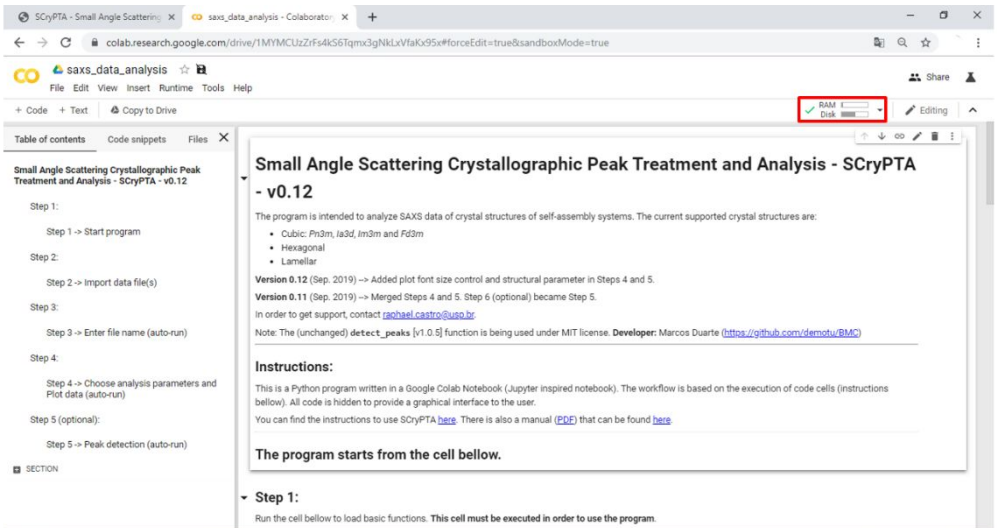
1) To start using the program, click at "OPEN IN PLAYGROUND" below the menu bar, as shown in the screenshot below:



2) Click at "CONNECT" in the right upper corner of the page:



3) The application will be ready to be used when the system status is displayed (see the red box in the screenshot):



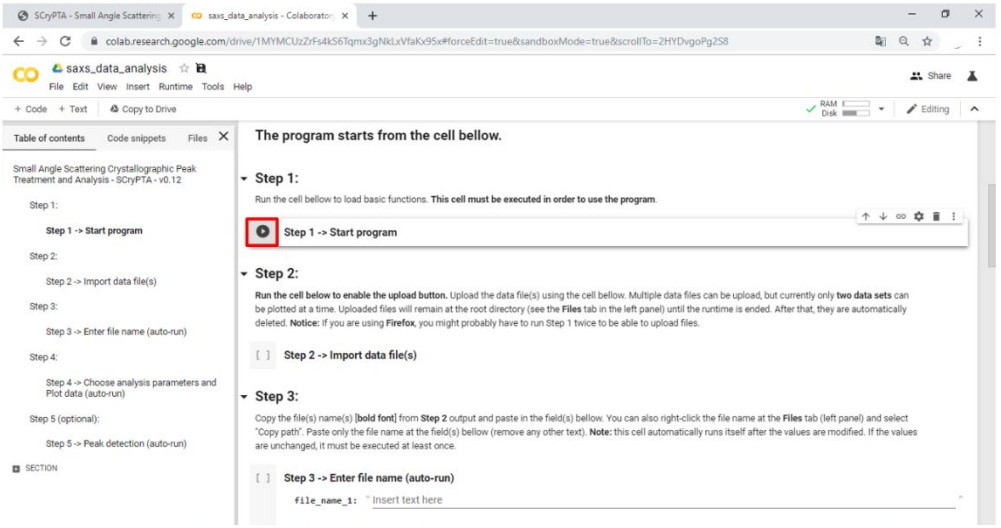
4) Each step (from 1 to 5) have instructions. Follow these instructions to execute each cell. After every modification, the cell must be executed.

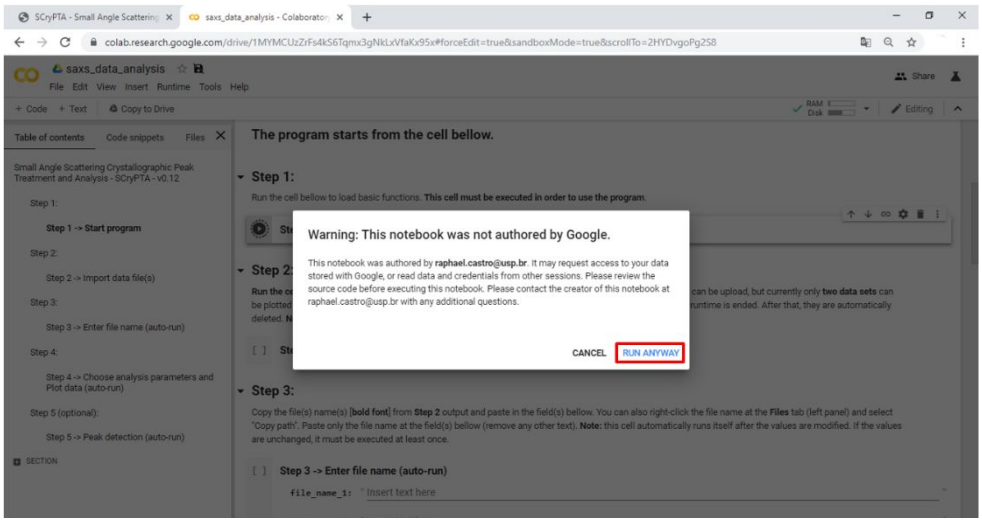
5) If the executed cell has no output, just run it once again.

6) Cells with auto-run feature must be executed by the user at least once after the program is initiated. From the first time, they will be executed automatically after any modification.

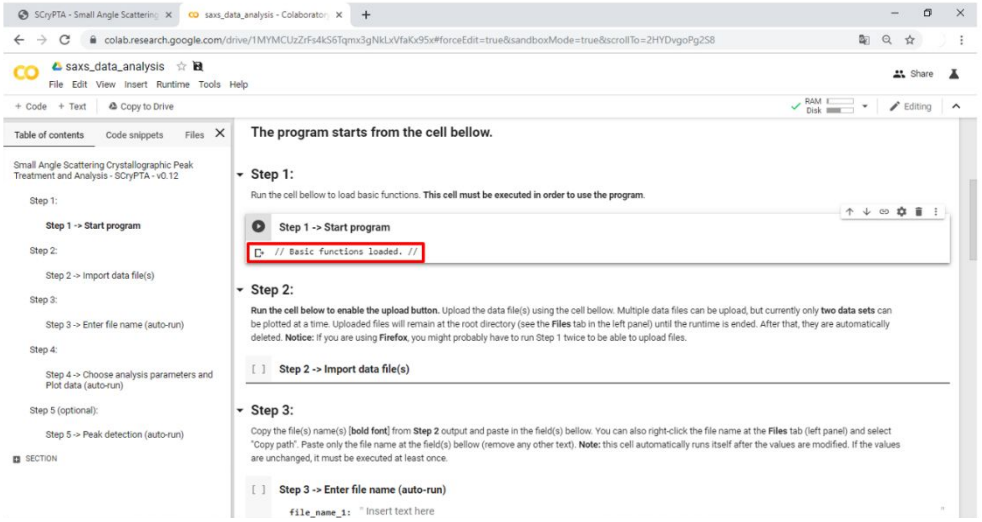
2- Data analysis

a) Step 1- Run the cell below to load basic functions**.** This cell must be executed in order to use the program. After this procedure, a screen for execution will appear. You must click on “RUN ANYWAY”.

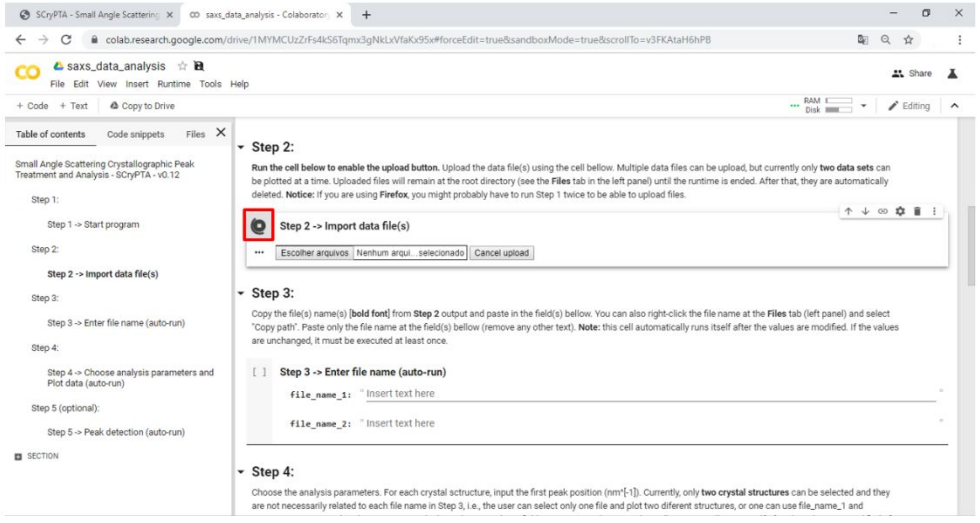




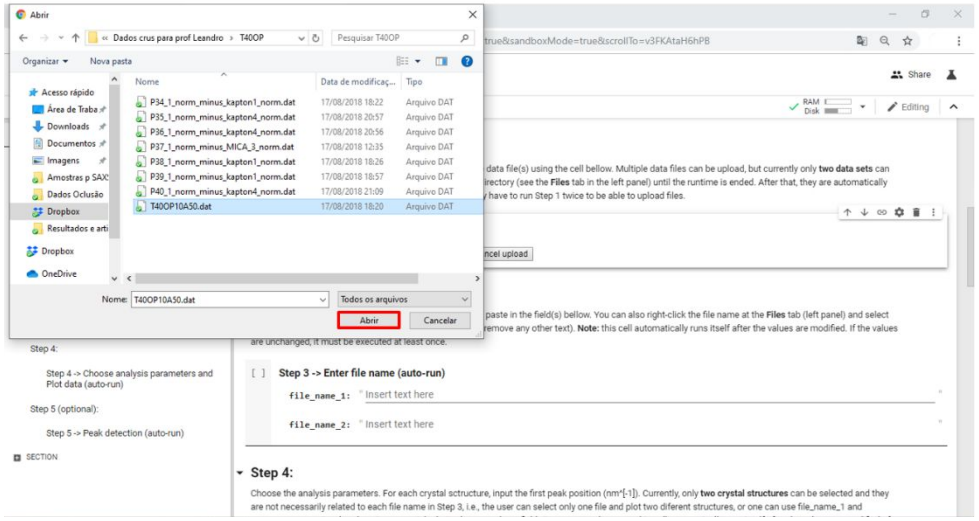
At the end of execution, the message "Basic functions loaded" will appear below Step 1:



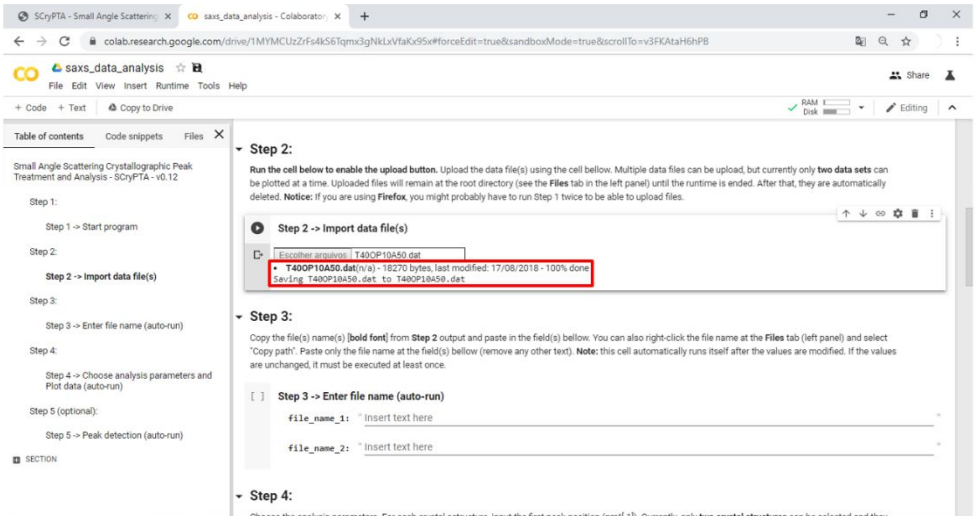
b) Step 2- Run the cell below to enable the upload button.



Upload the data file (s) using the cell. Multiple data files can be uploaded, but currently only two data sets can be plotted at a time.

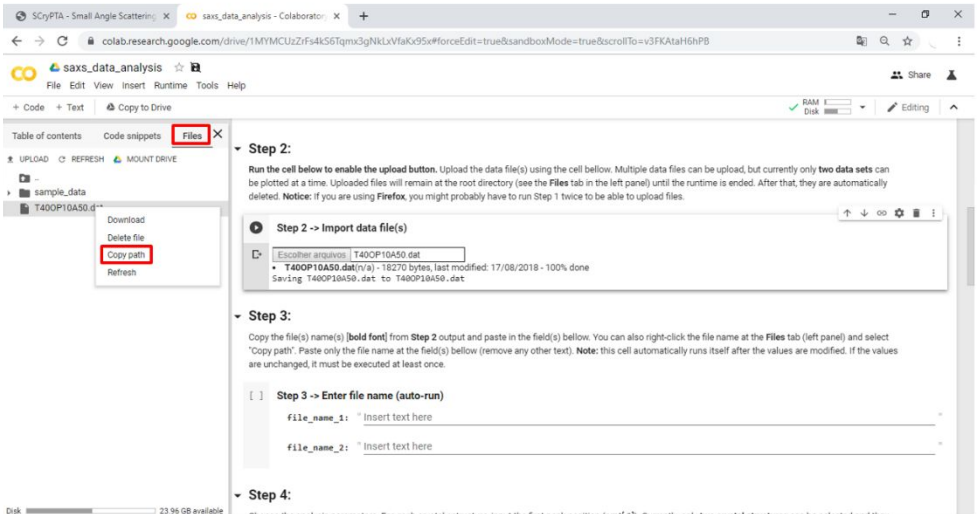


Once uploaded, it can be confirmed via the information below the cell:



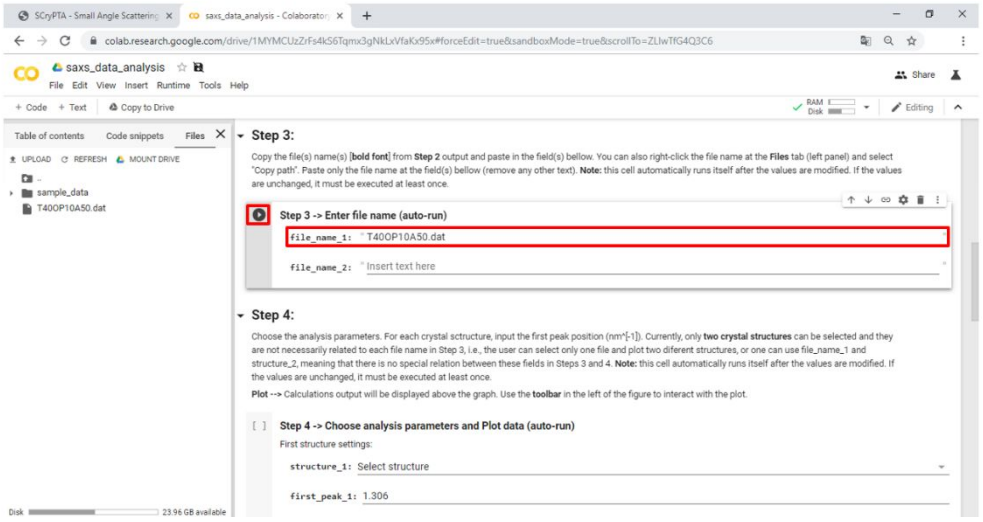
Multiple data files can be uploaded, but currently only two data sets can be plotted at a time. Uploaded files will remain at the root directory (see the Files tab in the left panel) until the runtime is ended. After that, they are automatically deleted. Notice: If you are using Firefox, you might probably have to run Step 1 twice to be able to upload files.

c) **Step 3-** Copy the file(s) name(s) [bold font] from Step 2 output and paste in the field(s) bellow. You can also right-click the file name at the Files tab (left panel) and select "Copy path".

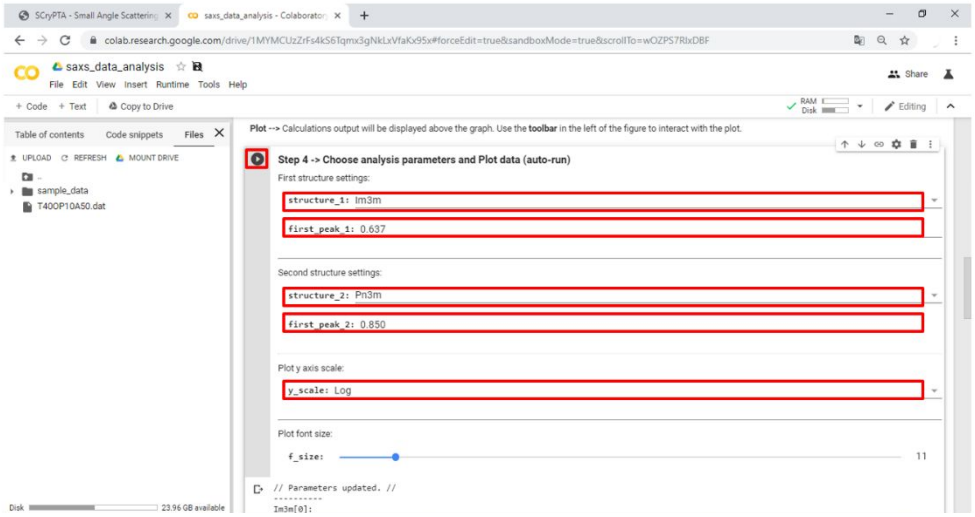


Paste only the file name at the field(s) bellow (remove any other text).

Note: This cell automatically runs itself after the values are modified. If the values are unchanged, it must be executed at least once.



d) **Step 4-** Choose the analysis parameters. For each crystal structure, input the first peak position (nm^[-1]). Currently, only two crystal structures can be selected and they are not necessarily related to each file name in Step 3, i.e., the user can select only one file and plot two different structures, or one can use **file_name_1** and **structure_2**, meaning that there is no special relation between these fields in Steps 3 and 4.



Note: this cell automatically runs itself after the values are modified. If the values are unchanged, it must be executed at least once.

Plot --> Calculations output are displayed above the graph. Use the **toolbar** on the left of the figure to interact with the plot.

e) **Step 5 (optional)-** Use a peak detection tool calculate other physical parameters. The output provides a calculated value for the first diffraction peak. You may use this value in **Step 4**. Paste the file name on the "file_name" field.