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 (<u>https://github.com/demotu/BMC</u>).

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

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Small Angle Scattering Crystallographic Peak Treatment and Analysis - SCryPTA - v0.12	Small Angle Scattering Crystallographic Peak Treatment and Analysis - SCryPTA		
Step 1:	- 00.12		
Step 1 -> Start program	The program is intended to analyze SAXS data of crystal structures of self-assembly systems. The current supported crystal structures are:		
Step 2:	Cubic: Prism, Ia3d, Im3m and Pd3m Hexagonal Lamellar		
Step 2 -> Import data file(s)	Version 0.12 (Sep. 2019)> Added plot font size control and structural parameter in Steps 4 and 5.		
Step 3	Version 0.11 (Sep. 2019) →> Merged Steps 4 and 5. Step 6 (optional) became Step 5.		
	In order to get support, contact raphael.castro@usp.br.		
Step 3 -> Enter file name (auto-run)	Note: The (unchanged) detect_peaks [v1.0.5] function is being used under MIT license. Developer: Marcos Duarte (https://github.com/demotu/BMC)		
Step 4:			
Step 4 > Choose applying parameters and	Instructions:		
Plot data (auto-run)	This is a Python program written in a Google Colab Notebook (Jupyter inspired notebook). The workflow is based on the execution of code cells (instructions bellow). All code is hidden to provide a graphical interface to the user.		
Step 5 (optional):	You can find the instructions to use SCryPTA here. There is also a manual (PDF) that can be found here.		
Step 5 -> Peak detection (auto-run)	The program starts from the cell bellow.		
	▼ Step 1:		
	Run the cell bellow to load basic functions. This cell must be executed in order to use the program.		

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".



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

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Step 3:		 Step 2. But the cell below to enable the unload button. Unload the data file(s) using the cell below. Multiple data files can be unload, but currently only two data sets can 		
Step 3 -> En	iter file name (auto-run)	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		
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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.

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

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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.

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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.

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