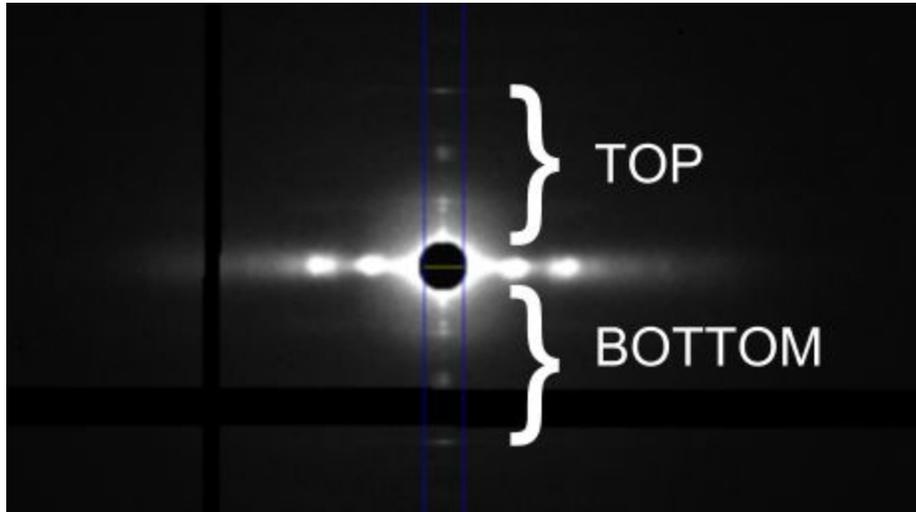


Diffraction Centroids

The objective of this program is to find the information of each diffraction from top part and bottom part of the frames after average and rotation.

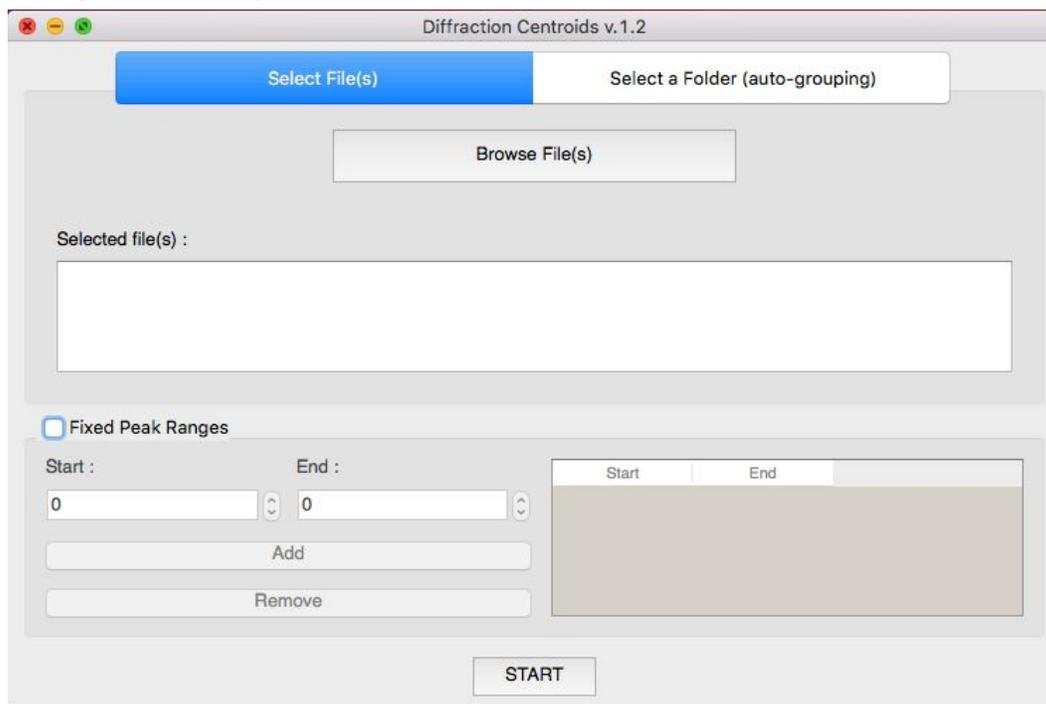


HOW TO USE

The program using is separated into 3 phases : Input, Image processing, and Diffractions

1. Input

After the program started, you will see this window below.



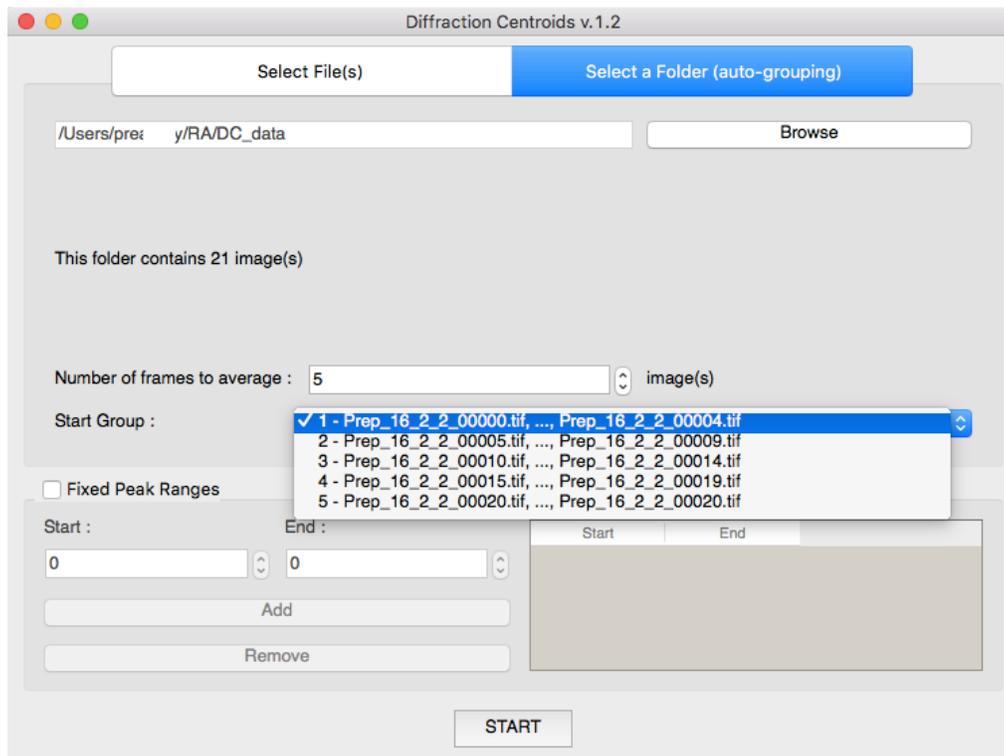
There are 2 types of input method, Files and Folder (Select by clicking the option on tab bar)



1.1 Select File(s) : This option will let you select a file or multiple files to average manually. The GUI will be the same as image above. To select files, you have to click on Browse File(s) button. Then, the input file dialog will be popped up. You can select multiple file by using Ctrl or Shift key with clicking. After files has been selected, the program will display number of files and name of files you selected.



1.2 Select a Folder (auto-grouping) : This option will let you select a folder and select number of frames to average, then , the program will group the images alphabetically automatically. First, You have to select a folder by clicking Browse button. After a folder selected, the program will display number of files in that folder. Then, you have to specify number of frames to average (Default : 5). The program will group the images alphabetically. For example, after a folder selected, you will see something like image below. At the Start Group drop down list, you will see start image name and end image name of each group. You can select a group to be the first group to process when START clicked



After you selected the input files or a folder already, now you can fix the position ranges of diffraction peaks (distance from the center in pixel) if you know them before processing by checking “Fixed Peak Ranges”. This will be unchecked by default. For example, if I know that the image will have peaks at around 30, 54, 82, 107, I can add all ranges by specify start and end of each range and click Add like below.

Fixed Peak Ranges

Start : End :

| | Start | End |
|---|-------|-----|
| 1 | 25 | 35 |
| 2 | 50 | 60 |
| 3 | 77 | 85 |
| 4 | 100 | 110 |

(You can remove the range by clicking on that row and click Remove)
 Finally, click START button to go to the next phase, Image processing.

2. Image processing

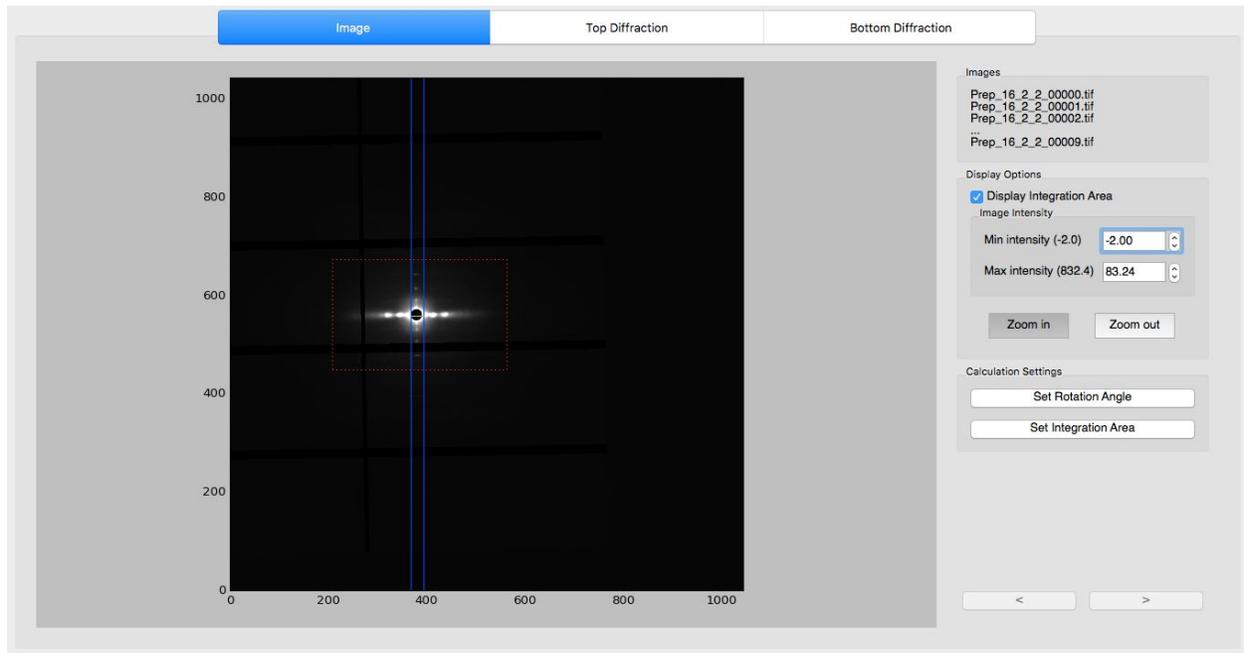
After START clicked, you will that there are 3 tabs on the top : Image, Top Diffraction, and Bottom Diffraction. In this phase, we are talking about the first tab which is Image tab. This phase will let you see the rotated average image, center, and the integration area.

The screenshot shows the 'Image' tab selected. The main display area shows a diffraction pattern with a vertical blue line at approximately x=400. The axes are labeled from 0 to 1000. On the right side, there are three sections: 'Images' (listing files like Prep_16_2_2_00000.tif), 'Display Options' (with 'Display Integration Area' checked and intensity sliders set to -2.00 and 83.24), and 'Calculation Settings' (with buttons for 'Set Rotation Angle' and 'Set Integration Area').

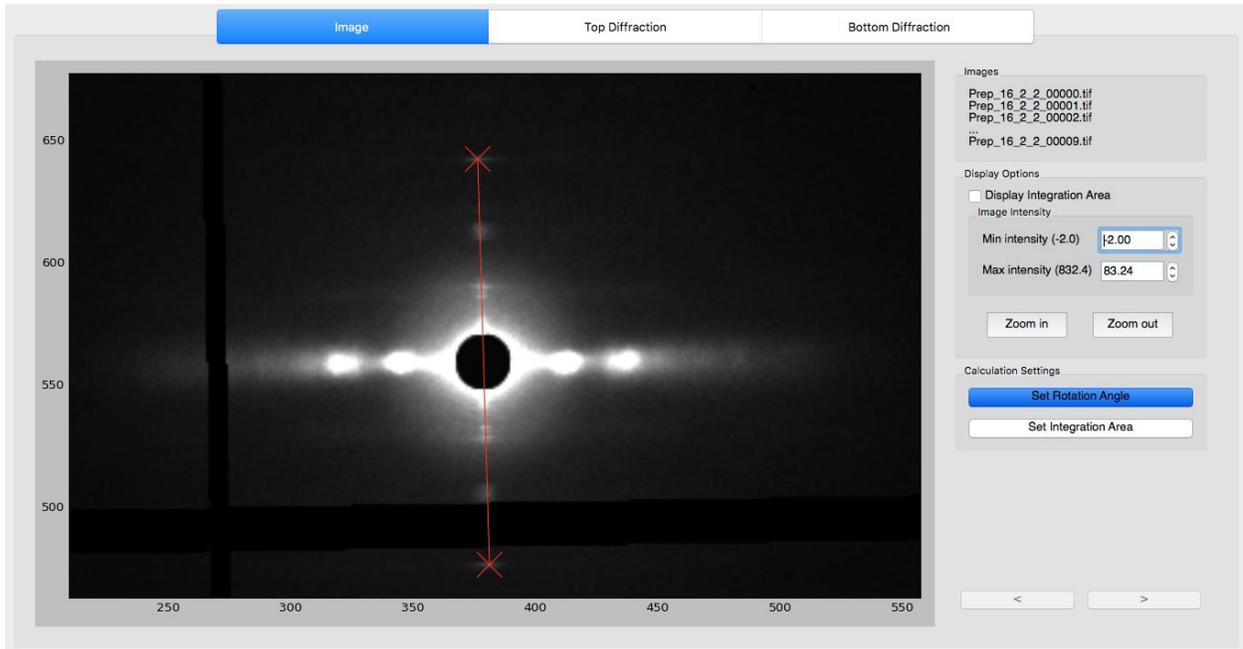
There are 3 sections on the right.

- Images : Names of image which are averaged

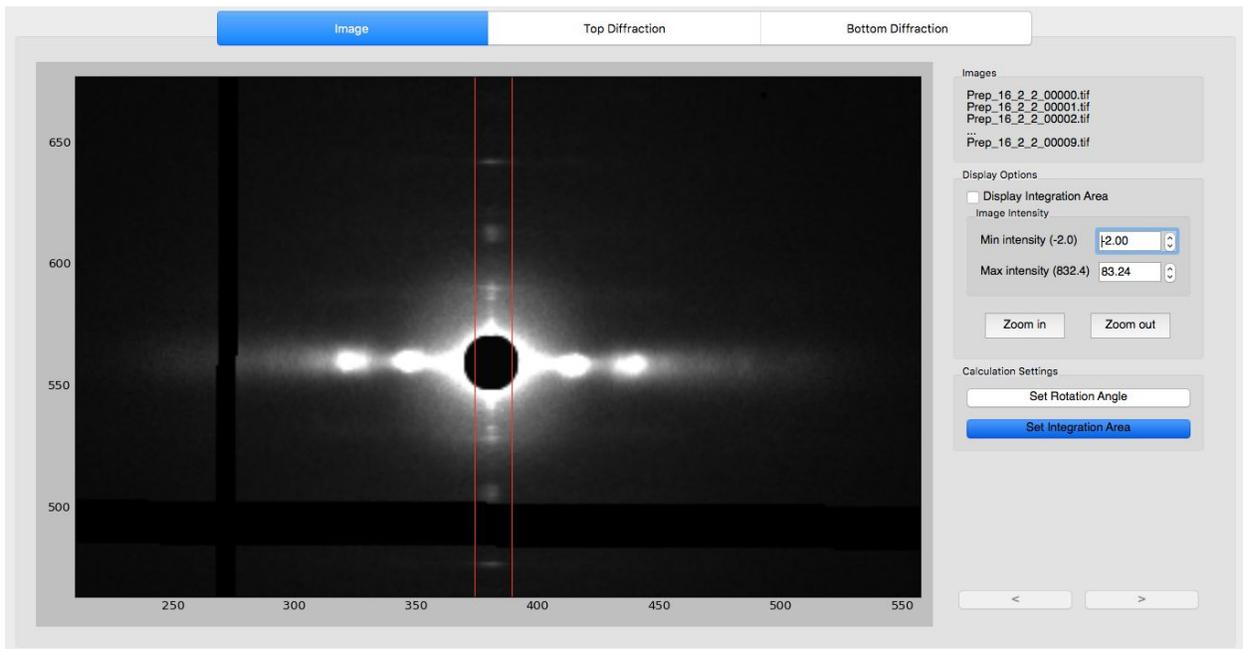
- Display Options : If you want to see the integration area and its center, you can check “Display Integrate Area” in this section. You can specify min and max intensity, so you can see the image clear. Also, you can Zoom in by clicking the Zoom in button and select the zoom in area on the image. To zoom out, just simply click Zoom out button. (This won’t affect the calculation part)



- Calculation Settings : You can select the rotation angle and integration area manually in case the program calculated them incorrectly. To select a new rotation angle, click “Set Rotation Angle”, then select a top diffraction and a corresponding bottom diffraction on the image. (You should zoom in the image before setting the rotation angle for the accuracy). This will manually set the rotation angle and its center, so please ensure that you pick the corresponding diffraction.



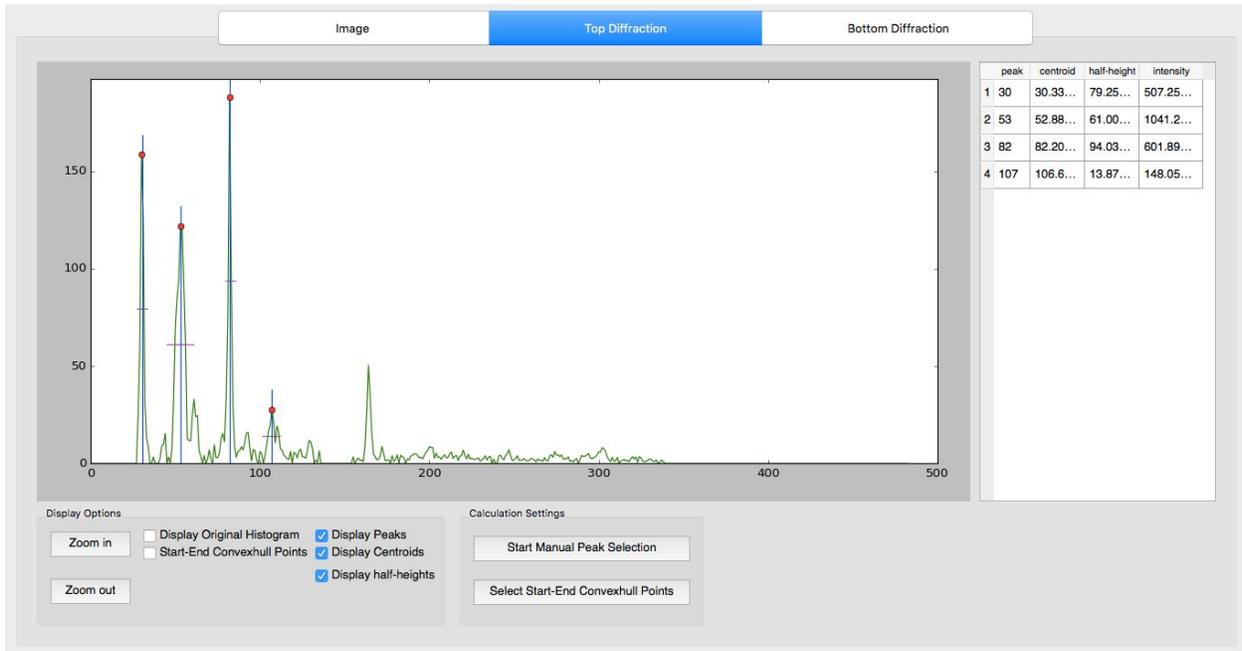
To Select the Integration Area, click “Set Integration Area”, and select the area by clicking on the image. You will see that the start and end of the area will be vertical lines, so make sure that you rotate the image properly before selecting the integration area.



3. Diffractions

After the image processing phase has been done, the program will find the histogram from vertical projection in the integration area. Then, separate the histogram into 2 parts by its center. Those diffractions will be shown in Top and Bottom Diffraction Tabs respectively.

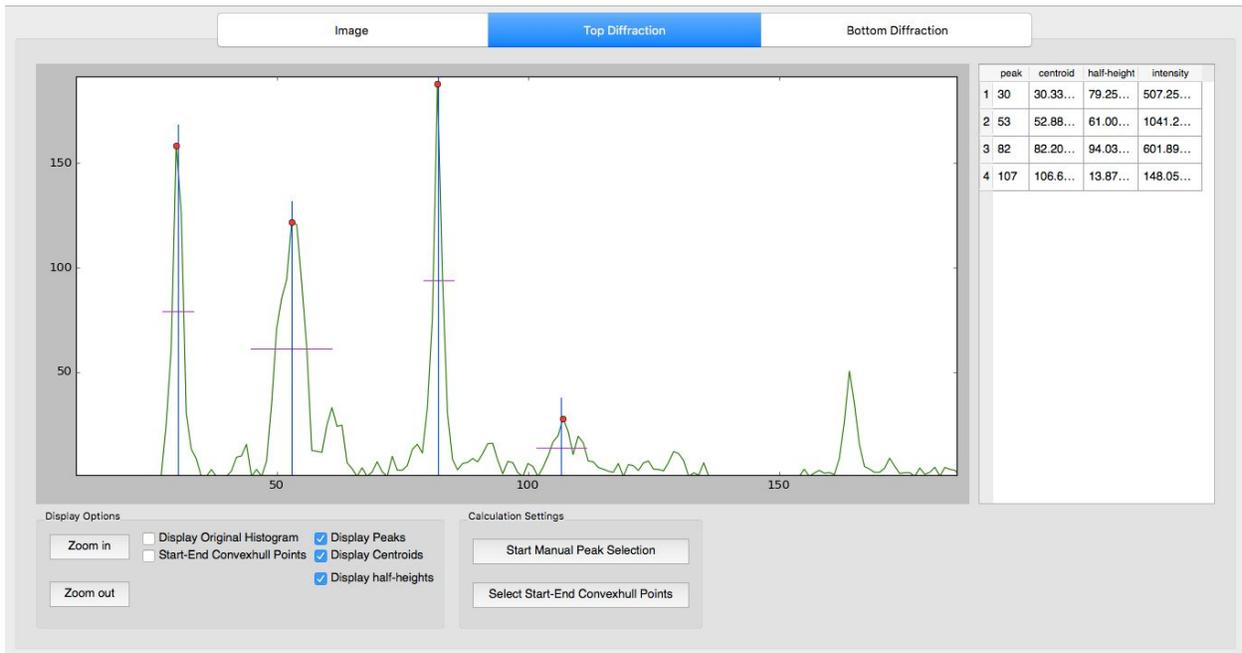
In the diffraction tab, you will see the histogram, option menu at the bottom, and peaks information in the table on the right as below.



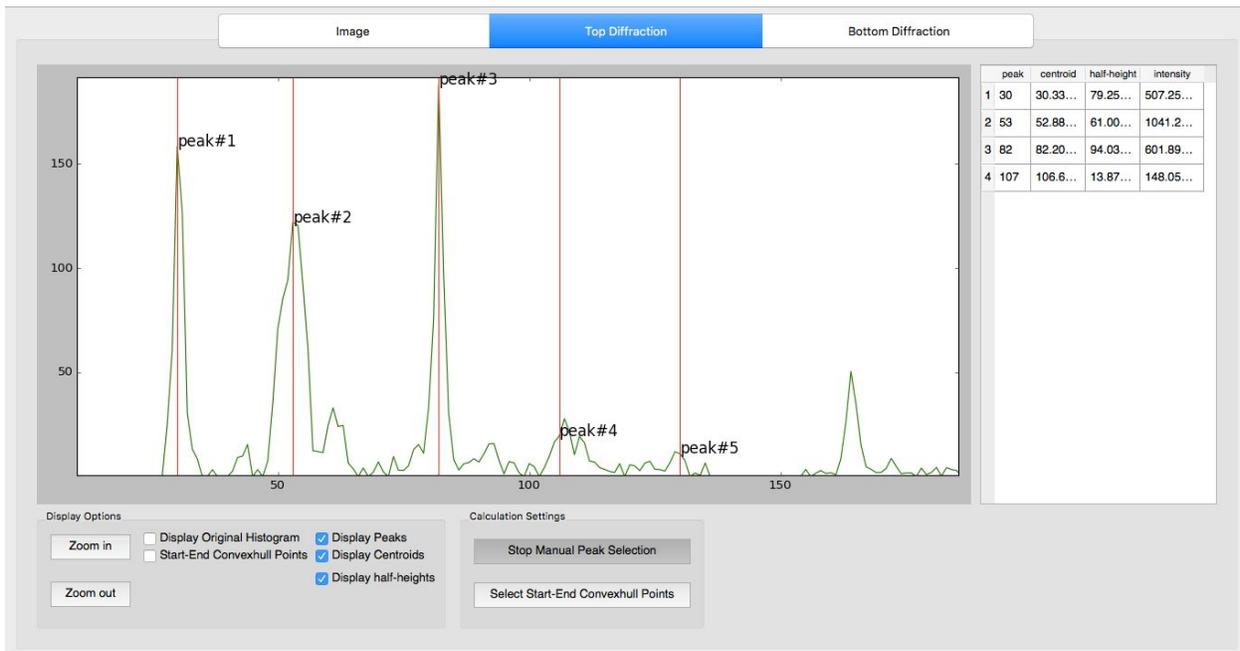
(In this case there are 4 peaks because we specify fixed peak ranges before the image processed)

For the option menu, there are 2 sections.

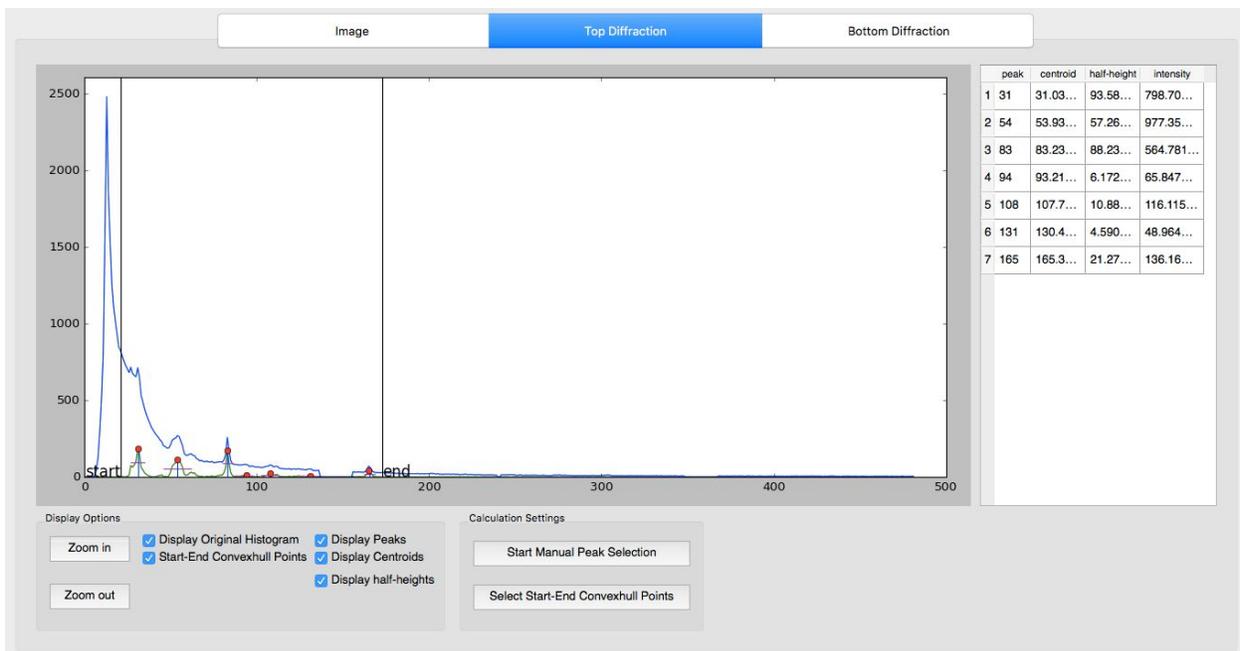
- Display Options : You can zoom in, zoom out, or display information to the plot by checking options provided. (This won't affect the calculation)



- Calculation Settings: You can select peaks manually by clicking on Start Manual Peak Selection, and click Stop Manual Peak Selection when you finished the selection.



You can also specify start and end convexhull points (for background subtraction) by clicking Start Start-End Convexhull Points. Then, select it on the plot.



Results

In the data folder, Diffraction Centroids will create a folder, summary. Inside the summary folder, you will see summary_m.csv if you select input files manually, and summary_fn.csv if you select

a folder with n frames auto-grouping. In the summary file, it contains group number, filenames, integration area width and peak informations as below

| group | filename | integration area width | side | peak | centroid | halfheight | intensity |
|-------|-----------------------|------------------------|---------------|---------------|---------------|---------------|---------------|
| 1 | Prep_16_2_2_00005.tif | 20 | top | 30 | 30.4421936626 | 85.3322892677 | 546.176171286 |
| | Prep_16_2_2_00006.tif | | top | 54 | 52.8434150108 | 64.163894818 | 958.267712221 |
| | Prep_16_2_2_00007.tif | | top | 82 | 82.2563872825 | 94.8151070023 | 606.871707849 |
| | Prep_16_2_2_00008.tif | | top | 107 | 106.572857766 | 14.4487516773 | 154.133992707 |
| | Prep_16_2_2_00009.tif | | bottom | 31 | 30.7538497424 | 69.6452213941 | 594.35977785 |
| | Prep_16_2_2_00010.tif | | bottom | 53 | 53.1117576989 | 52.5858915383 | 785.353852388 |
| | Prep_16_2_2_00011.tif | | bottom | 82 | 82.3397878986 | 86.0470067782 | 550.750778118 |
| 2 | Prep_16_2_2_00012.tif | 21 | top | 30 | 30.4927406104 | 47.1206397896 | 301.599439669 |
| | Prep_16_2_2_00013.tif | | top | 53 | 52.748145923 | 71.5765033057 | 1221.68308902 |
| | | | top | 82 | 82.0587479836 | 105.35858495 | 449.57072353 |
| | | | top | 107 | 106.490985098 | 16.9694775051 | 108.614503748 |
| | | | bottom | 31 | 30.5093660941 | 96.1609042314 | 615.485591108 |
| | | | bottom | 54 | 53.0936284571 | 71.3667220056 | 913.576872642 |
| | | | bottom | 82 | 82.4230705254 | 80.140712534 | 512.947067419 |
| 3 | Prep_16_2_2_00000.tif | 18 | top | 30 | 30.3899216381 | 65.9049429144 | 421.829880562 |
| | Prep_16_2_2_00001.tif | | top | 53 | 52.8842845905 | 58.2432112486 | 994.107604398 |
| | Prep_16_2_2_00002.tif | | top | 82 | 82.0664935038 | 91.2296509297 | 389.281805517 |
| | Prep_16_2_2_00003.tif | | top | 107 | 106.287515831 | 11.1996899116 | 143.369029661 |
| | Prep_16_2_2_00004.tif | | bottom | 30 | 30.6792088097 | 57.0088961641 | 364.890018812 |
| | | | bottom | 54 | 52.9715274992 | 51.7611009935 | 883.469558196 |
| | | | bottom | 82 | 82.3171652502 | 73.0799481385 | 467.75407779 |
| | bottom | 107 | 106.299934159 | 11.7563017012 | 150.494306593 | | |