

USER MANUAL



Designed and Developed by



INTRODUCTION

XPLOT v8.21 is one of the most useful software in the field of X-Ray Diffraction which is used for the processing of raw data. Its Graphic User Interface (GUI) contains all types of controls on single dashboard so its use is very simple. A person having little knowledge of computer can run this software without any hurdle and special training. XPLOT v8.21 contains its license embedded in hardware key which is supplied with the software. Updates are available for life time free of cost.

XPLOT v8.21 is the fastest software among XRD data processing software. One can complete all procedures and get printout of XRD pattern in 2 – 3 minutes including Baseline Straightening, Peak Stripping, data smoothing and Peak Search. XPLOT v8.21 has many practical features for other applications and presentations. Prominent features are Export Graph, Export ASCII data, Save Peak and Search Data, Custom Plotting and Multiple Graphs. Page orientation can be set as Portrait or Landscape and therefore printing can be done accordingly. The printout is obtained in the form of report which is highly stylish, presentable and contains all important information about XRD processed data. Multiple Graphs utility is also very useful program which is used to compare the XRD patterns and can also be used in research publications.

The determination of Particle Size is another important feature of XPLOT v.21. It uses most famous Scherrer Formula and calculates particle size in micro meter and nano meter scales. For higher accuracy data of 10 peaks can be entered and average value is calculated after each entry. In this way one can also find out the quality of its data which he measured on X-ray Diffractometer. XPLOT v8.21 can be used for XRD data collected using X-ray tube having Cu, Cr, Fe, Co, Mo and W targets.

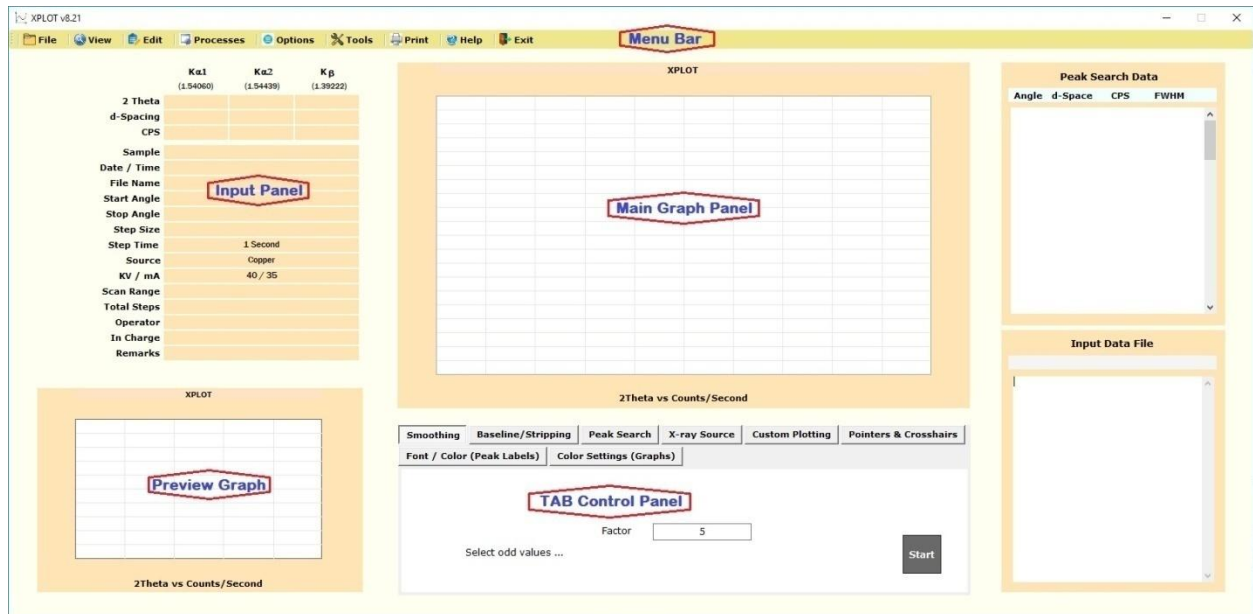
One can also customize Graphic User Interface for personal display and other applications. For instance one can change font, font style, background color and foreground color of peak labels, graphs and XY Scales according to his own choice. One can show and hide gridlines and peak labels for better visibility if data contains many overlapped peaks and noisy data. Pointers and crosshairs can also be displayed over graph area to find out peak angles and intensity levels of unlabeled peaks quickly with the help of tooltip message box.

A very important feature of data correction is also included in Default Settings. So you will get reliable output with 100% accuracy and precision. With this feature you have full control to correct the raw data. If XPLOT v8.21 is being used on Work Place you can clear the graph data before leave. This feature has its own importance if you don't want to disclose your work done for others. There are many other features which we can explore on your own.

XPLOT v8.21 accepts two columns ASCII data files with TAB space and XML files. In case of ASCII data files first column contains 2 Theta Angles and second column contains CPS. While in case of XML data it can accept XML file as document and extracts values of 2 Theta and CPS data automatically. We can customize XPLOT v8.21 for other input data formats on request. For more information about its applications and troubleshoots please visit www.hightechpakistan.com to find contact details.

XPLOT v8.21

Before operating the XPLOT v8.21 go through naming convention of different sections of its GUI.



Input Panel

Many text boxes of input panel are automatically filled when you import raw data file. All text boxes of input panel are editable and you can type details in the empty text boxes and edit filled text boxes also.

Main Graph Panel

The diffraction patterns of all imported 2 column ASCII data files, Raw data files, *.smo files, *.bal files, XML files and data with customized scales are displayed here.

Preview Graph

All files imported first time are displayed here for reference and comparison purpose.

TAB Control Panel

This panel contains 8 different TAB controls. You have options to enter the parametric values of different processes at one place.

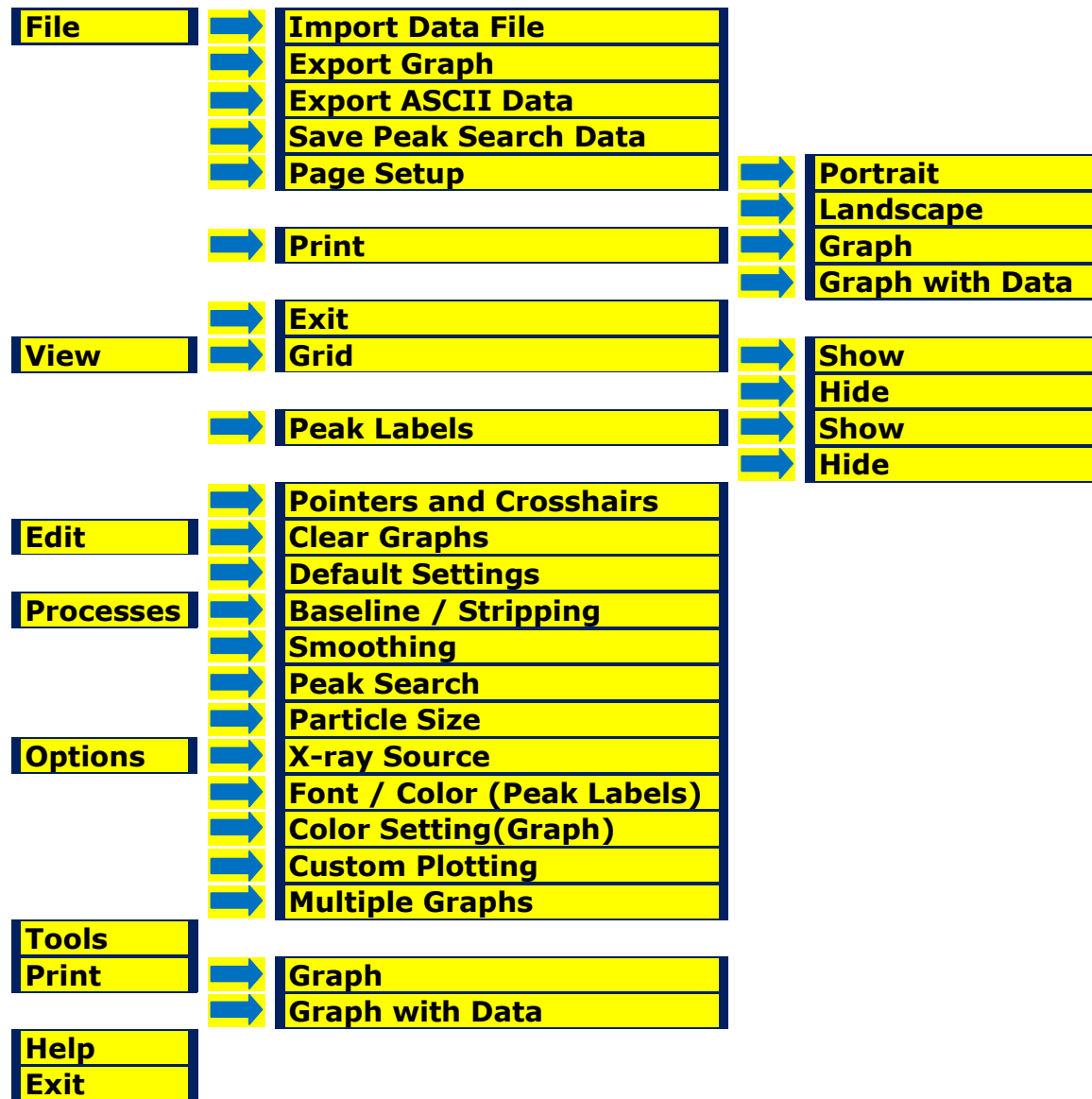
Peak Search Data

The output of Peak Search program is displayed here.

Input Data File

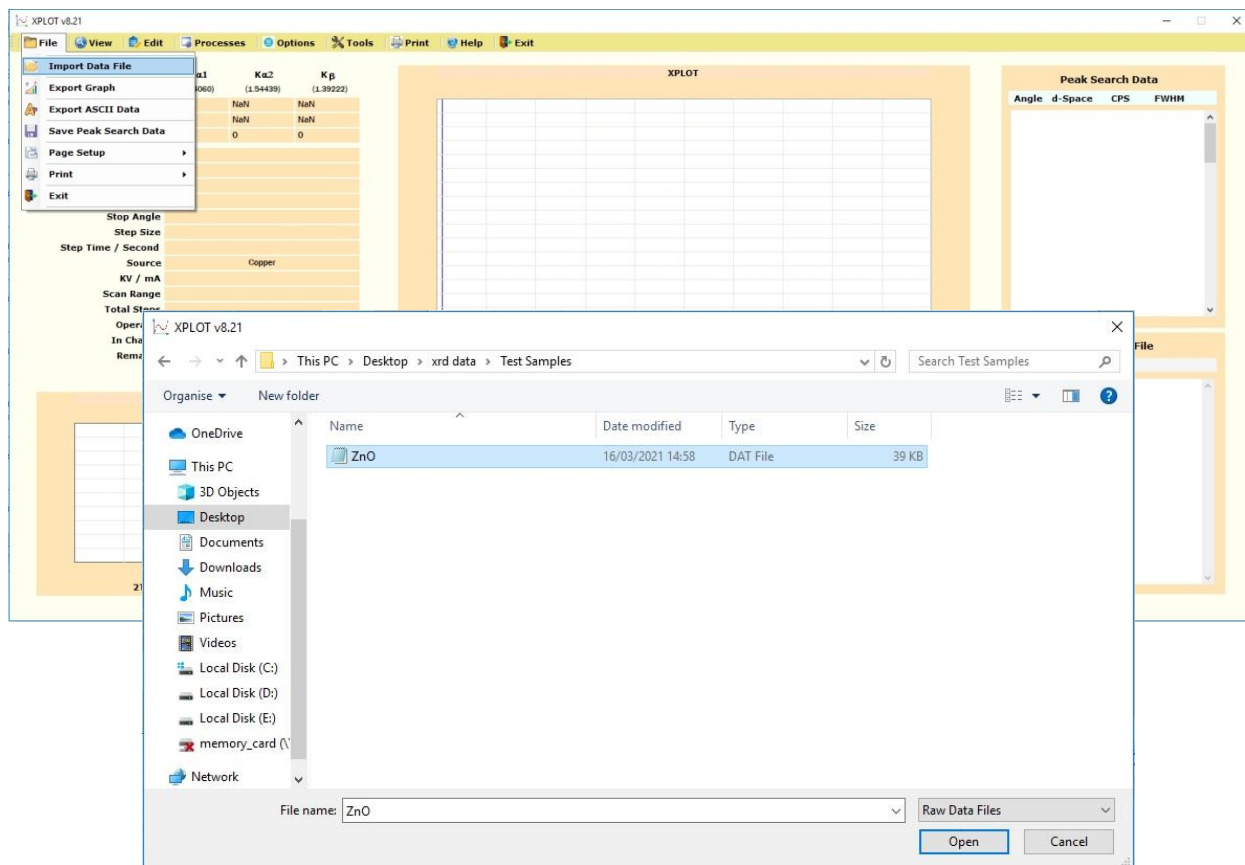
The contents of all imported and processed files are displayed here for quick check purpose.

Menu Bar Hierarchy



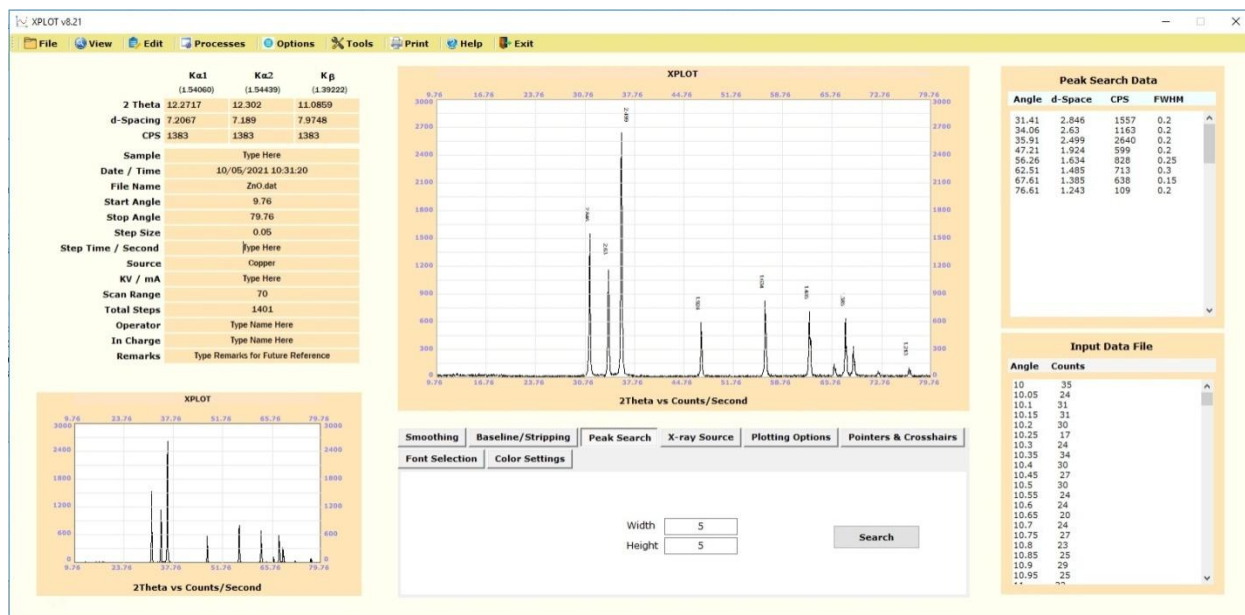
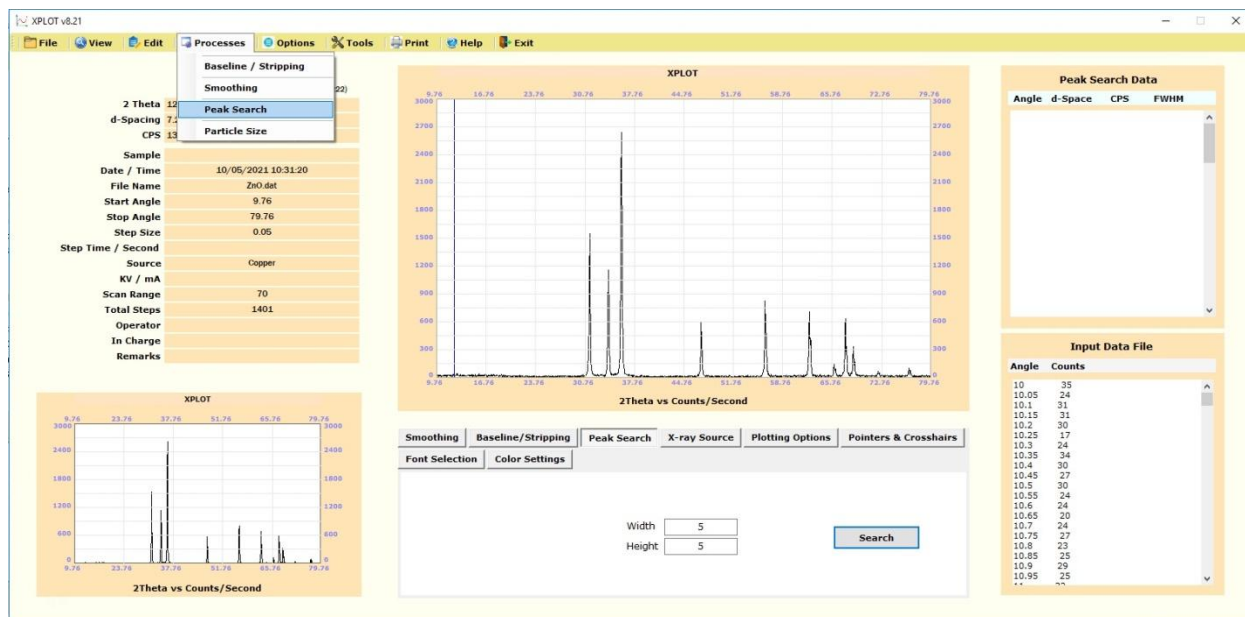
How to Import Data File and Plot

1. Clicking on **File** TAB, dropdown menu will be displayed
2. Click on **Import Data File**
3. Browse your file and click on **open** button in the open file dialog.



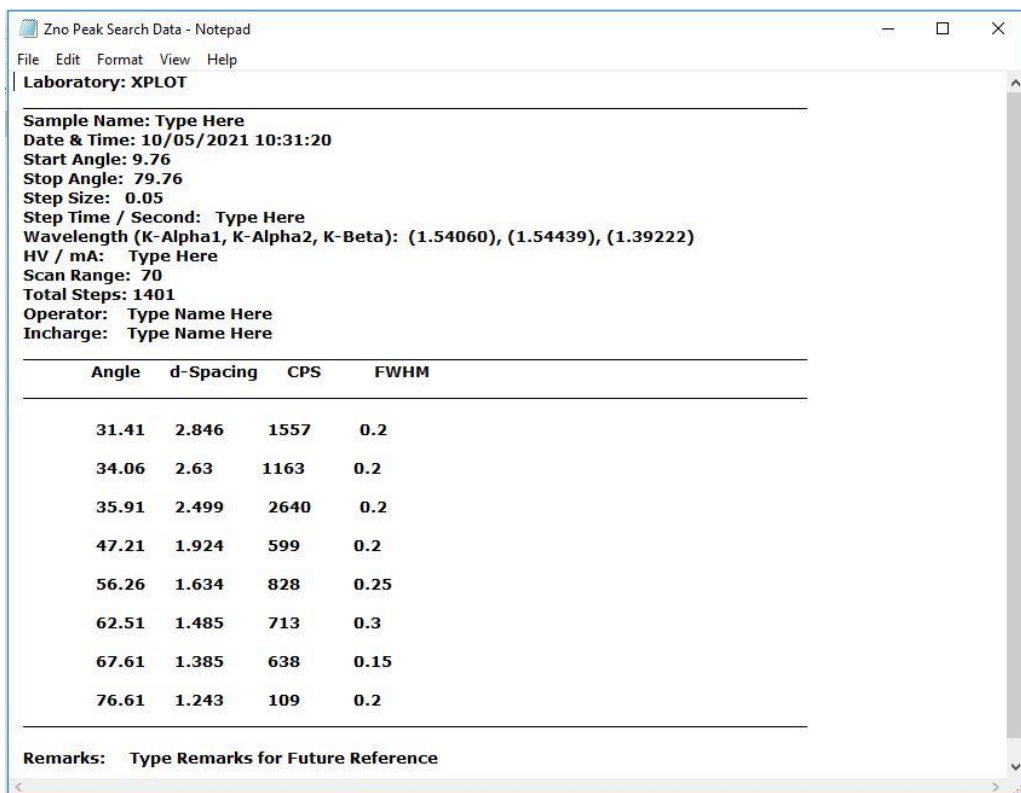
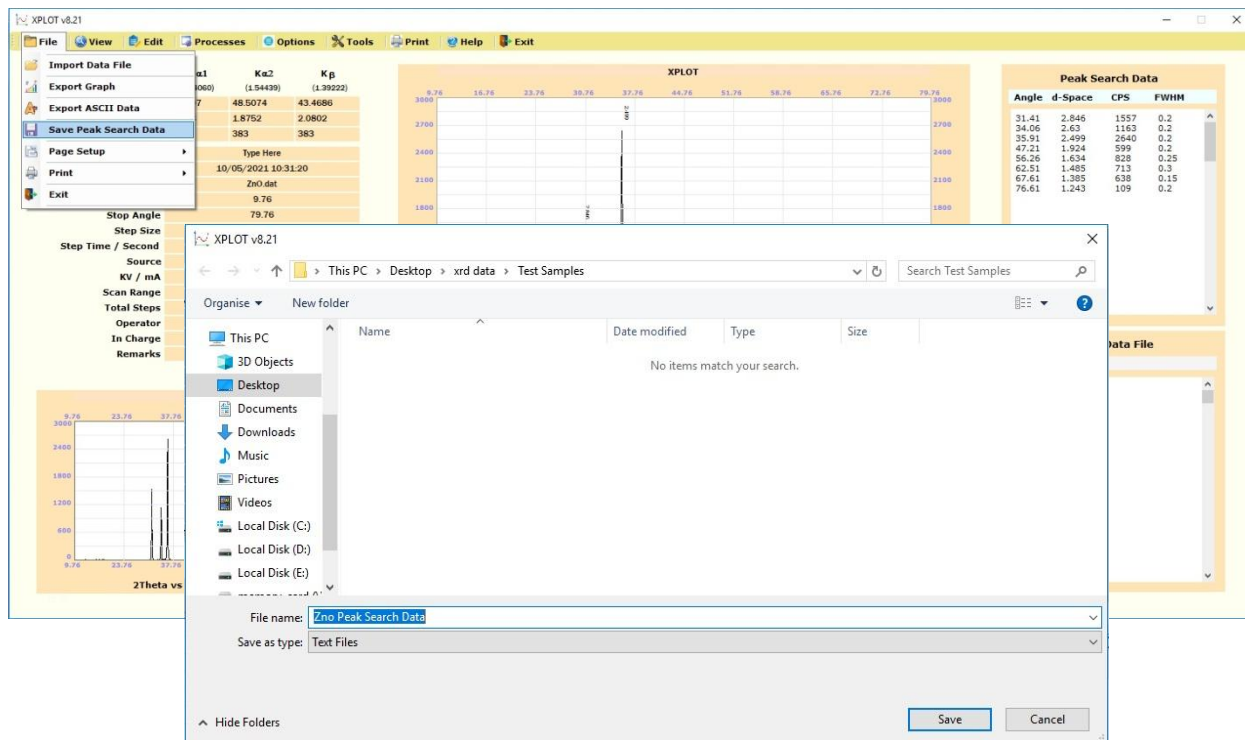
How to Search Peaks

1. Click on **Processes** TAB → Click on **Peak Search**
2. Change the arbitrary values of Width and Height in the TAB Control Panel or keep default values as it is. Default values are 5 and 5 which are suitable for most of the XRD patterns for phase analysis → Click on **Search** button.
3. Unlabelled peaks can be labeled by changing the arbitrary values of **Width** and **Height** of peaks. These are average arbitrary values applicable on all peaks so select the values accordingly.



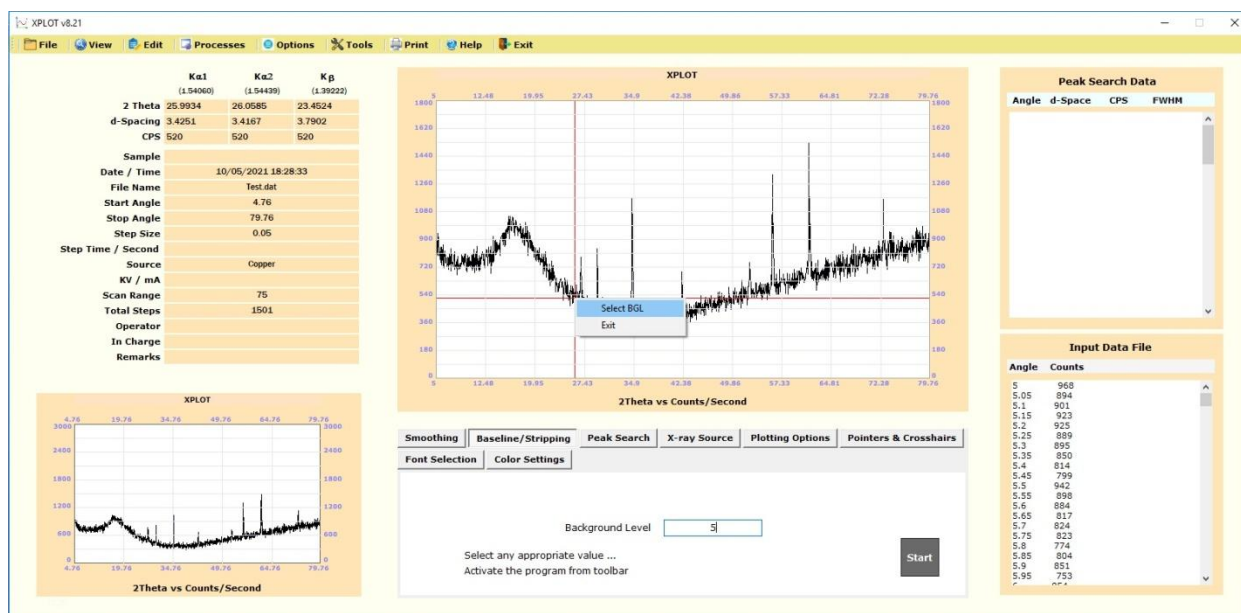
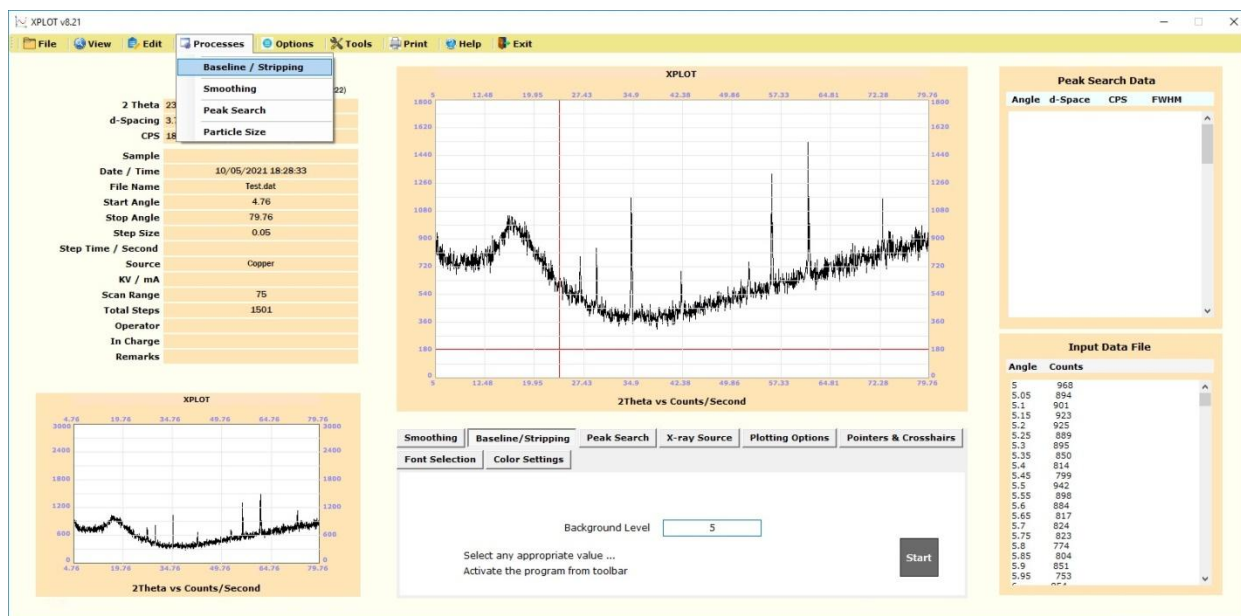
How to Save Peak Search Data in a File

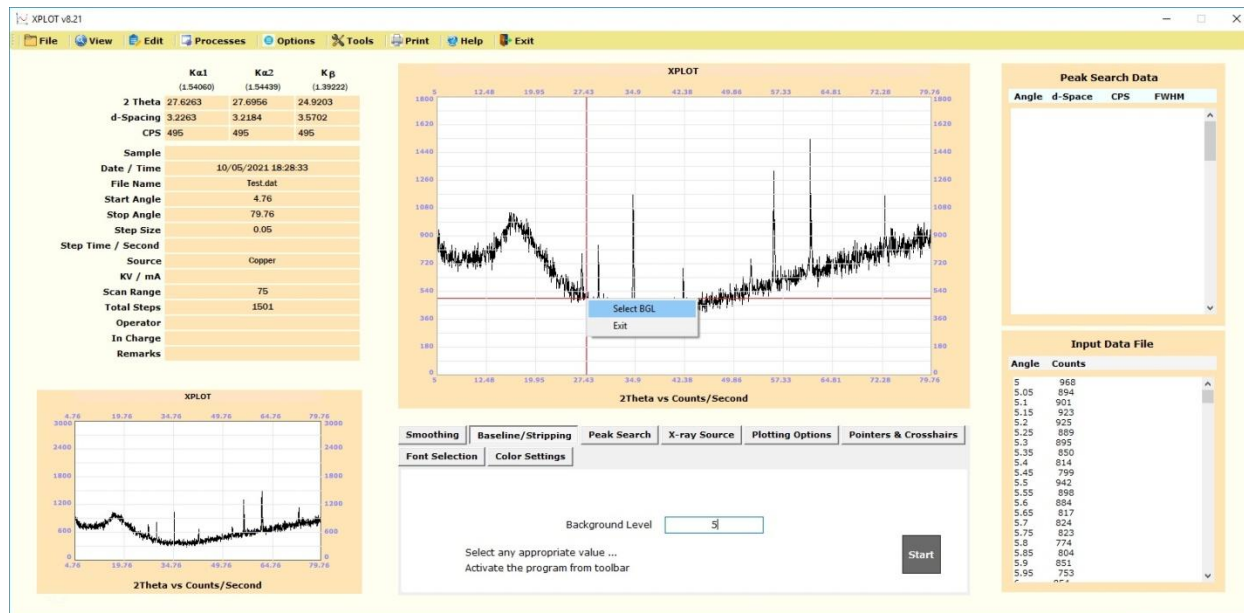
1. Click on **File** Tab → **Save Peak Search Data**
2. Type file name in the text box of save file dialog and click on **Save** button.



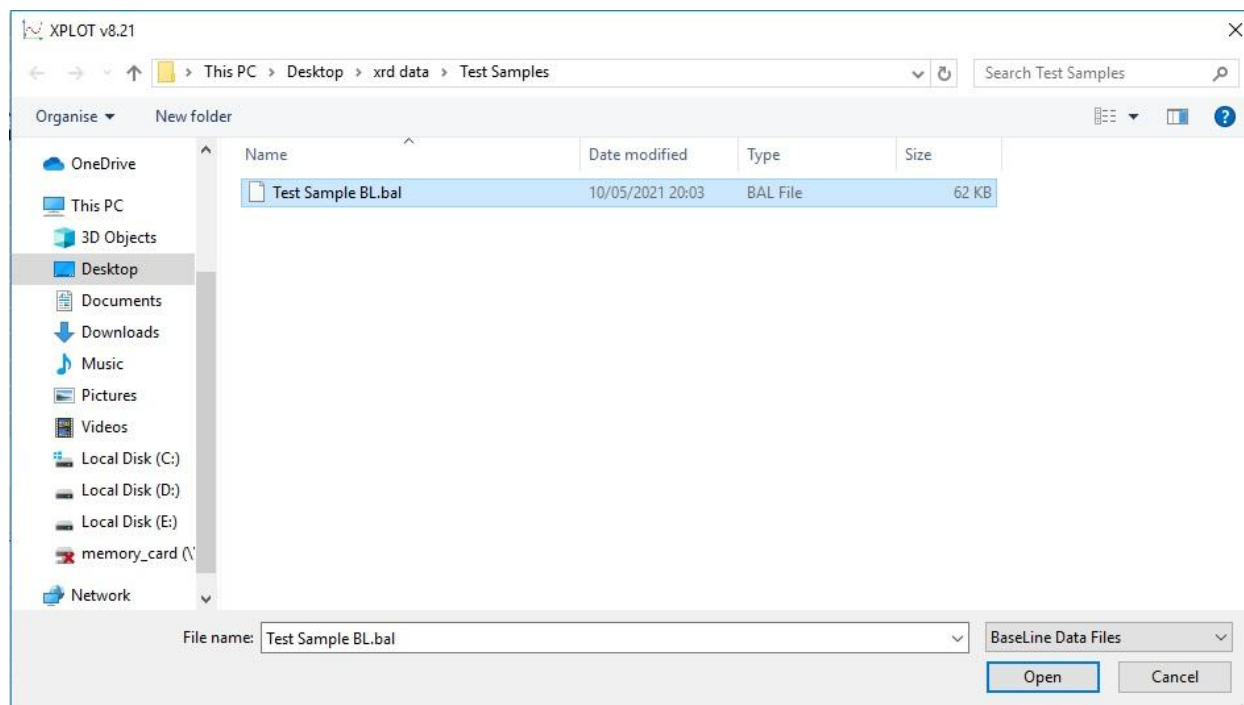
How to Straighten the Baseline and Stripping or Trimming the Undesired Peaks

1. Click on **Processes** TAB → Click on **Baseline / Stripping**
2. Baseline straightening and stripping of undesired peaks are done simultaneously. In this procedure backgrounds of left hand sides and backgrounds of right hand sides of those peaks are selected which are valid peaks. Move the mouse on the main graph area you will see crosshairs are appeared. Now bring the mouse pointer on left side of first valid peak and right click as shown in picture below. You will see pop-up menu and click on **Select BGL**. After that bring the mouse pointer on right side of first valid peak and right click. You will again see pop-up menu and click on **Select BGL**. (Best background level "BGL" is just before the start of peak and just after the peak where it ends as shown in picture)

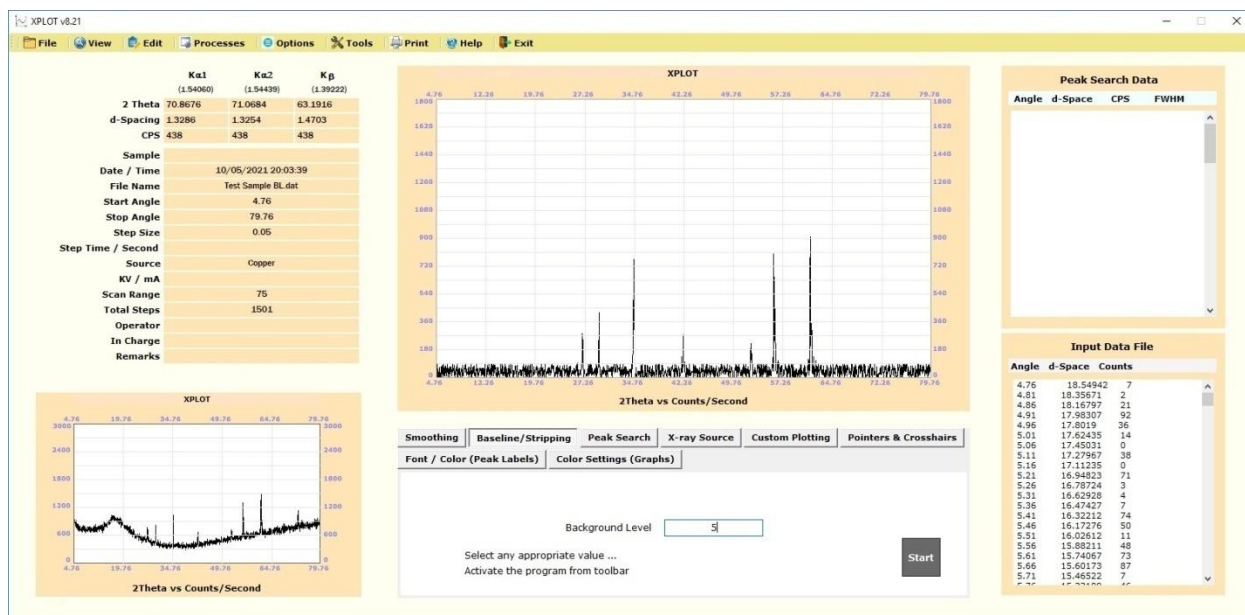




3. Repeat above mentioned procedure in serial 2 with all valid peaks.
4. Click on **Start** button shown in the TAB control Panel.

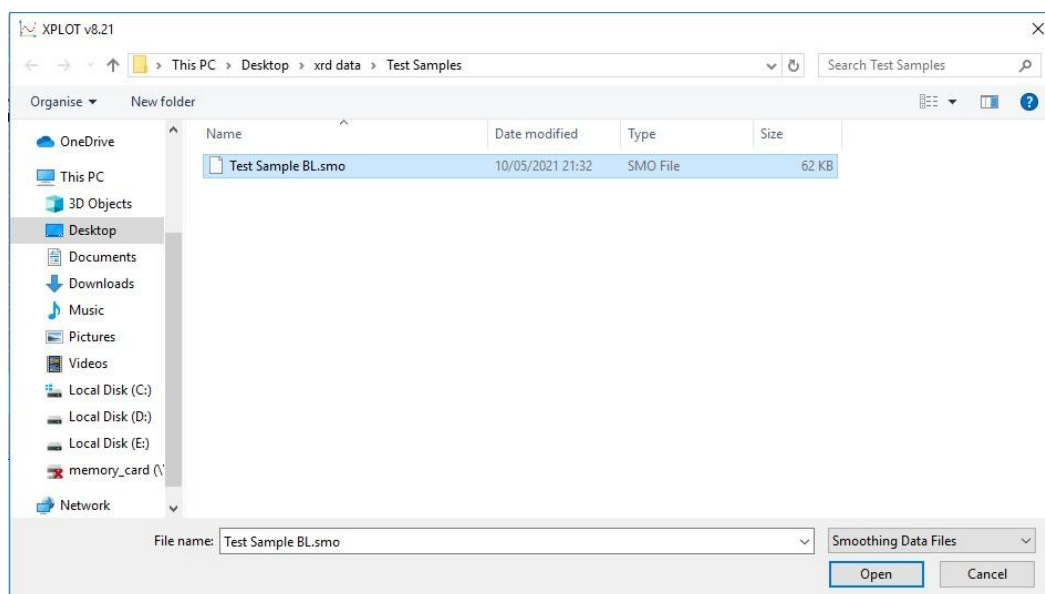


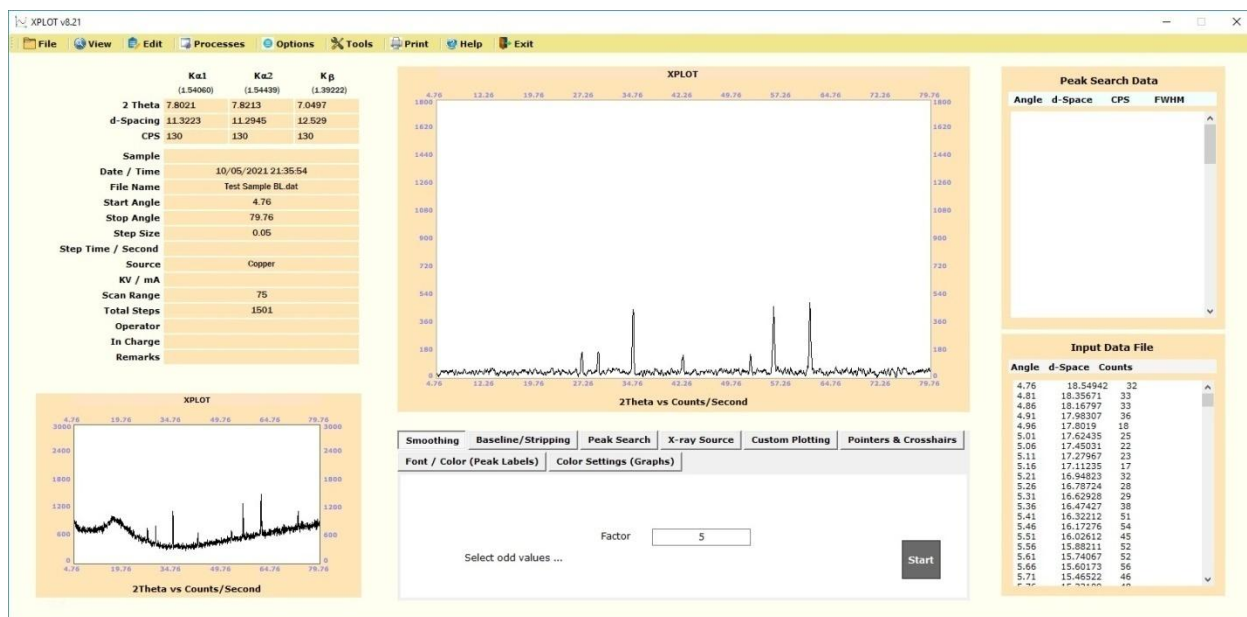
5. It will automatically show the open file dialog. Select the same file name which is now with new extension "bal" and click on **Open** button. You will immediately get the following graph with straightened background. The hump in pattern and other undesired peaks have been eliminated completely.



How to Smooth the XRD data

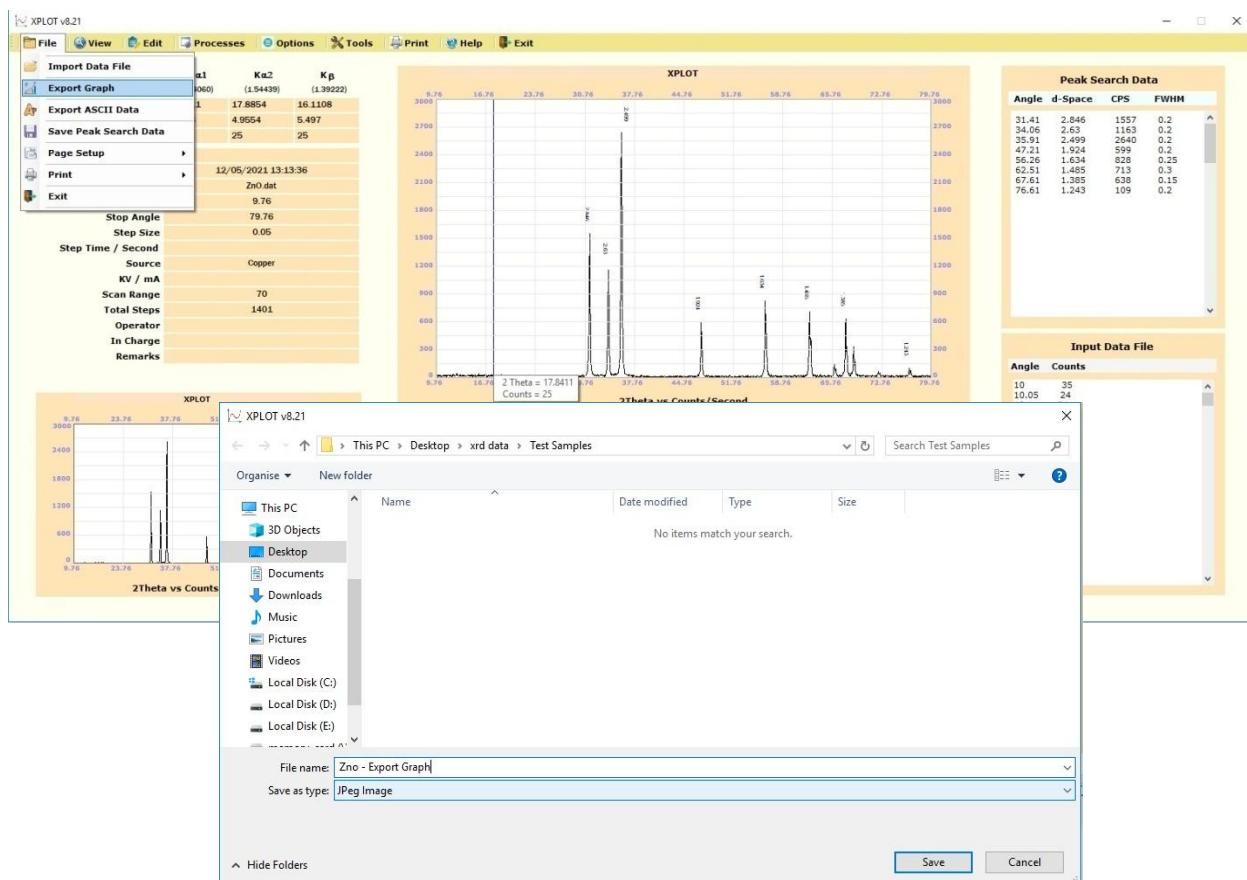
1. If you look the above graph background, you will find noise is quite high. Therefore to minimize the background noise smoothing of data is required. For this purpose you need smoothing of data. Hence click on **Processes** TAB → **Smoothing**
2. Now go to **Tab Control Panel** under the main graph. Enter some **odd value** in the factor text box. Default factor value is 5 and it is suitable for most of the patterns. Normally it is the ratio between the background level and background trimming level.
3. Clicking on **Start** button will show file open dialog box
4. Select the same file name in the Open File Dialog but with new extension "**smo**" and click on the **Open** button to get final result.

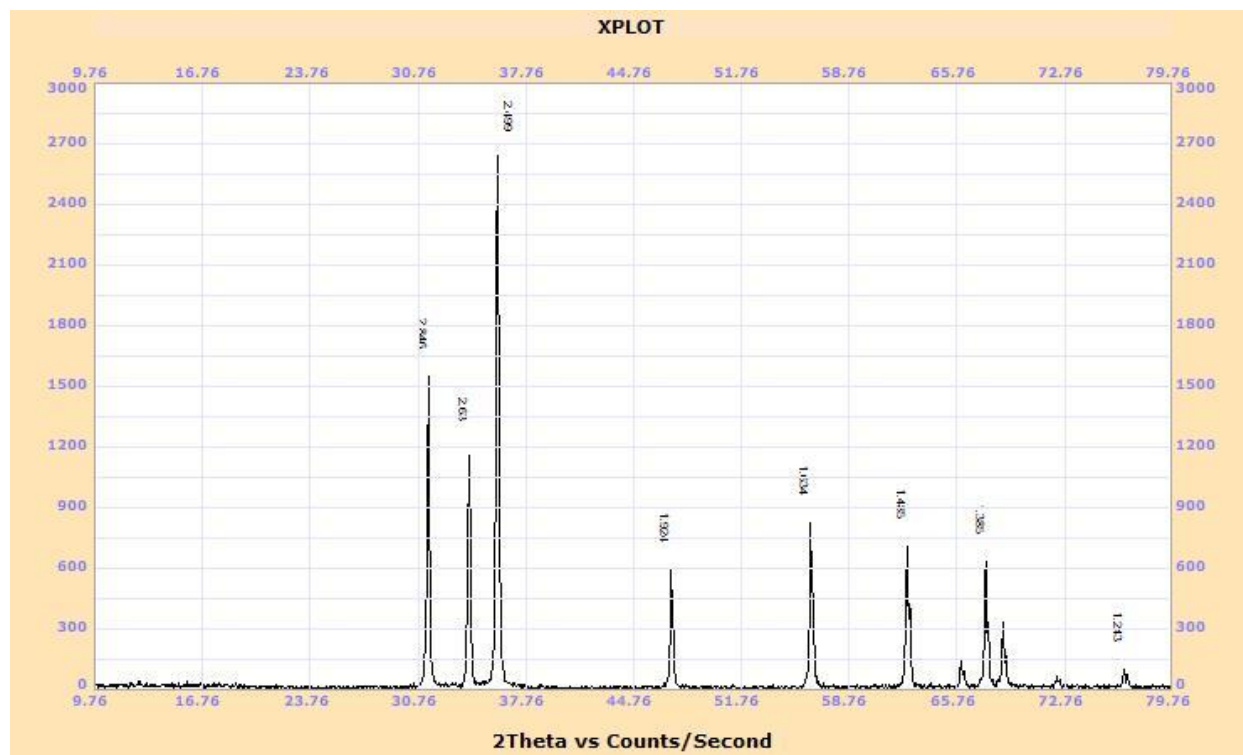




How to Export Graph as Image File

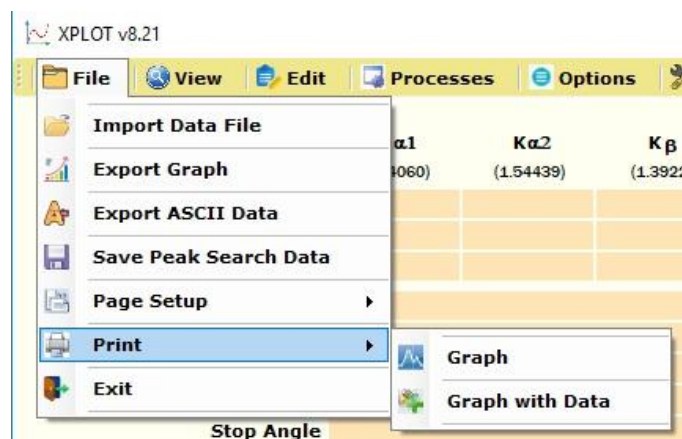
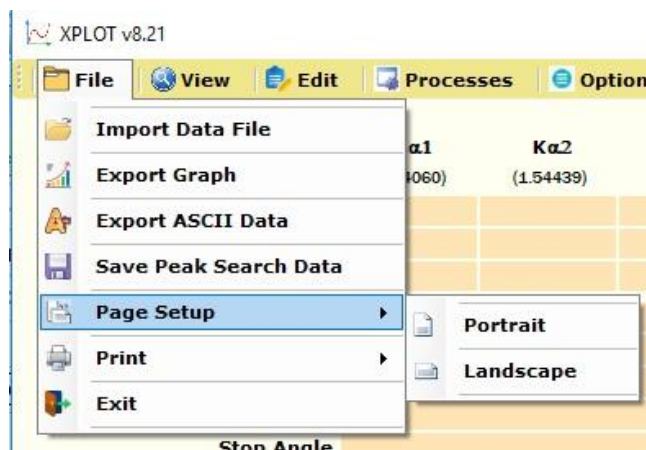
1. Click on **File** TAB → Click on **Export Graph**
2. Type file name in the text box of Save File Dialog and click on **Save** button.



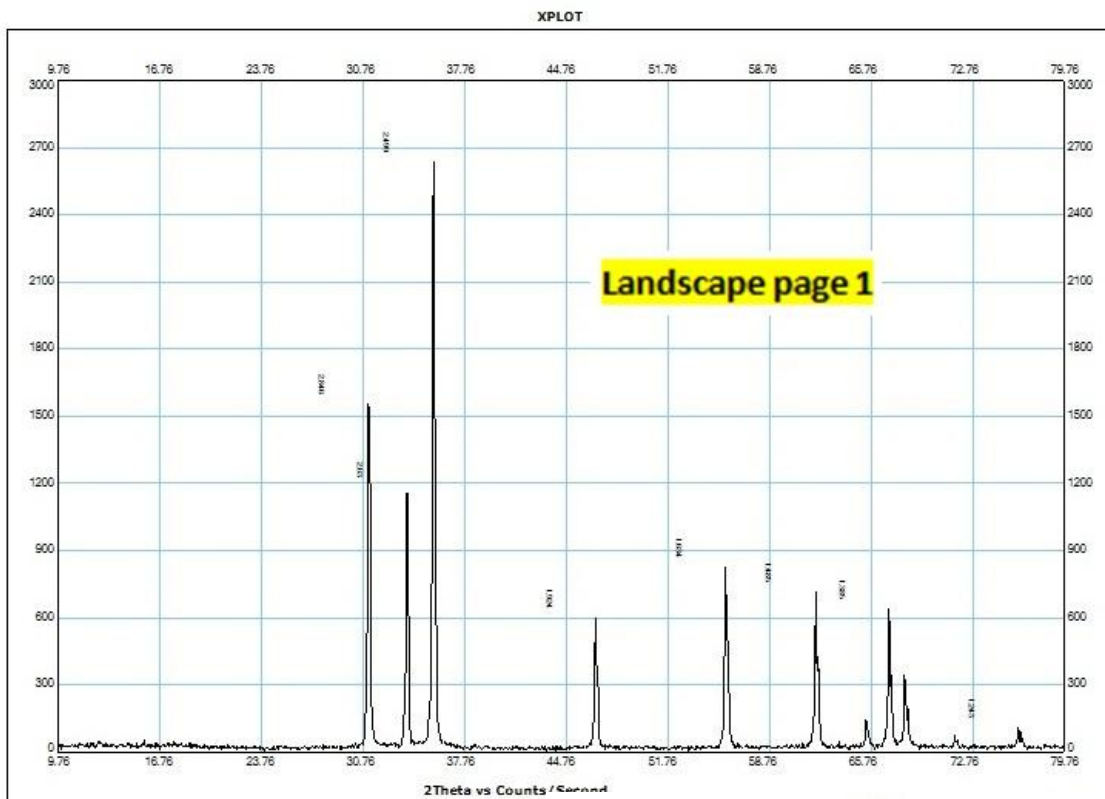


Printing of Graph and Results

Before clicking on Print command select first page orientation in the **Page Setup** menu where you have two options "**Portrait**" and "**Landscape**". Similarly you have two options in the Print menu; "**Graph**" and "**Graph with Data**". In case of Portrait and Landscape page setup "**Graph with Data**" will print on one and two pages respectively. Default option is Portrait.

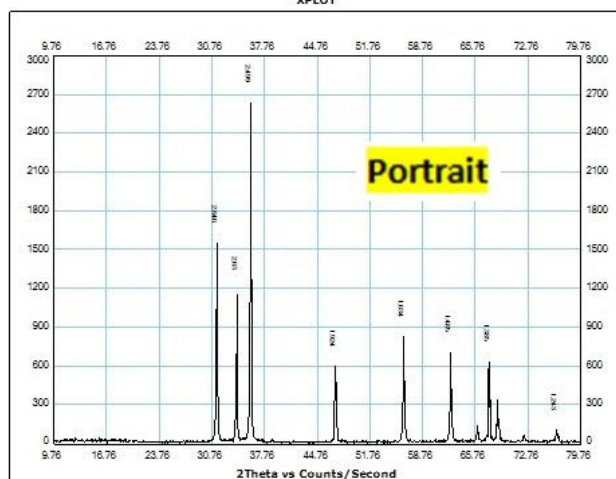


See the Printouts on next page.



Sample					Source	1.5406					
Date / Time	07:21:12 13/05/2021				KV / mA						
File Name	ZnO.dat				Scan Range	70					
Start Angle	9.76				Total Steps	1401					
Stop Angle	79.76				Operator						
Step Size	0.05				In Charge						
Step Time					Remarks						
Angle	Spacing	CPS	FWHM	Angle	Spacing	CPS	FWHM	Angle	Spacing	CPS	FWHM
31.41	2.846	1557	0.2								
34.06	2.63	1163	0.2								
35.91	2.489	2640	0.2								
47.21	1.924	599	0.2								
56.26	1.634	828	0.25								
62.51	1.485	713	0.3								
67.61	1.385	638	0.15								
76.61	1.243	109	0.2								

Landscape page 2

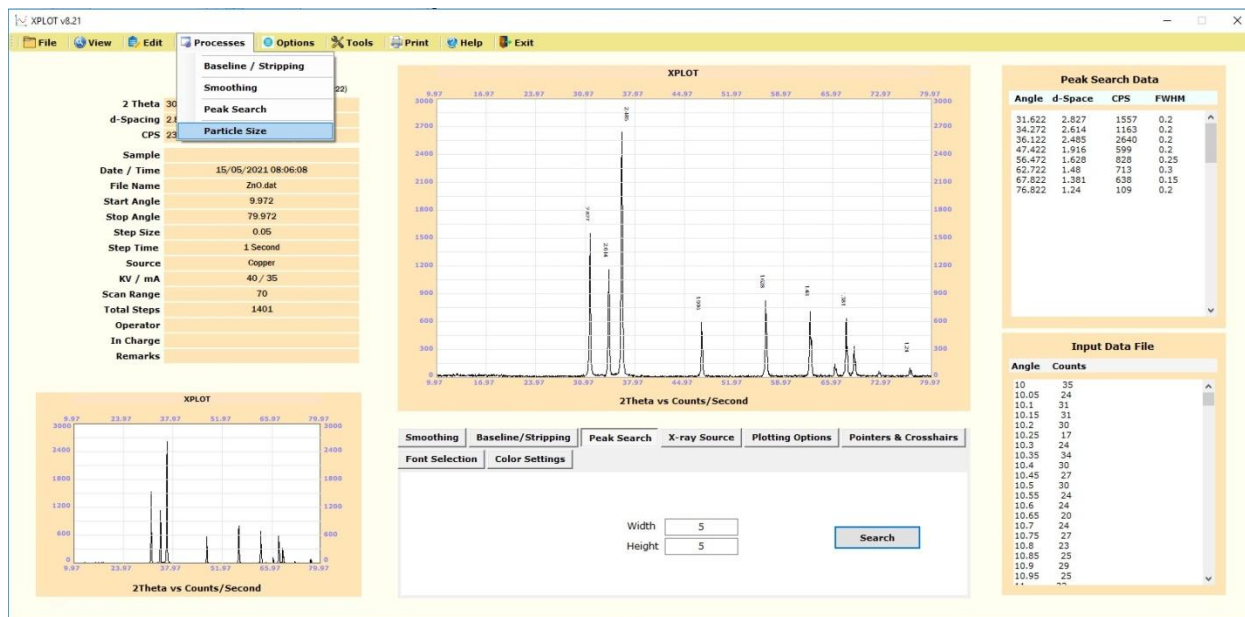


Sample		Source		Copper			
Date / Time		KV / mA					
File Name		Scan Range		70			
Start Angle		Total Steps		1401			
Stop Angle		Operator					
Step Size		In Charge					
Step Time		Remarks					
Angle	Spacing	CPS	FWHM	Angle	Spacing	CPS	FWHM
31.41	2.846	1557	0.2				
34.06	2.63	1163	0.2				
35.91	2.489	2640	0.2				
47.21	1.924	599	0.2				
56.26	1.634	828	0.25				
62.51	1.485	713	0.3				
67.61	1.385	638	0.15				
76.61	1.243	109	0.2				

How to Measure Particle Size

This program measures particle size using Scherrer Formula. For better result enter data of all peaks or maximum 10 peaks. In column 3 you find the results of individual peak and in column 4 you find the average results of all preceding peaks. Select scale micrometer or nanometer before start.

Procedure is very simple. Enter peak angle and FWHM in the corresponding text boxes and click on **Proceed** button. Repeat this procedure for all valid peaks up to maximum 10 peaks. You can save and print the results for future use.



XPLLOT v8.21

New Save Data Print Exit

Estimation of Particle Size

Display Scale ☐ Nanometer ☒ Micrometer

Specimen

Date / Time

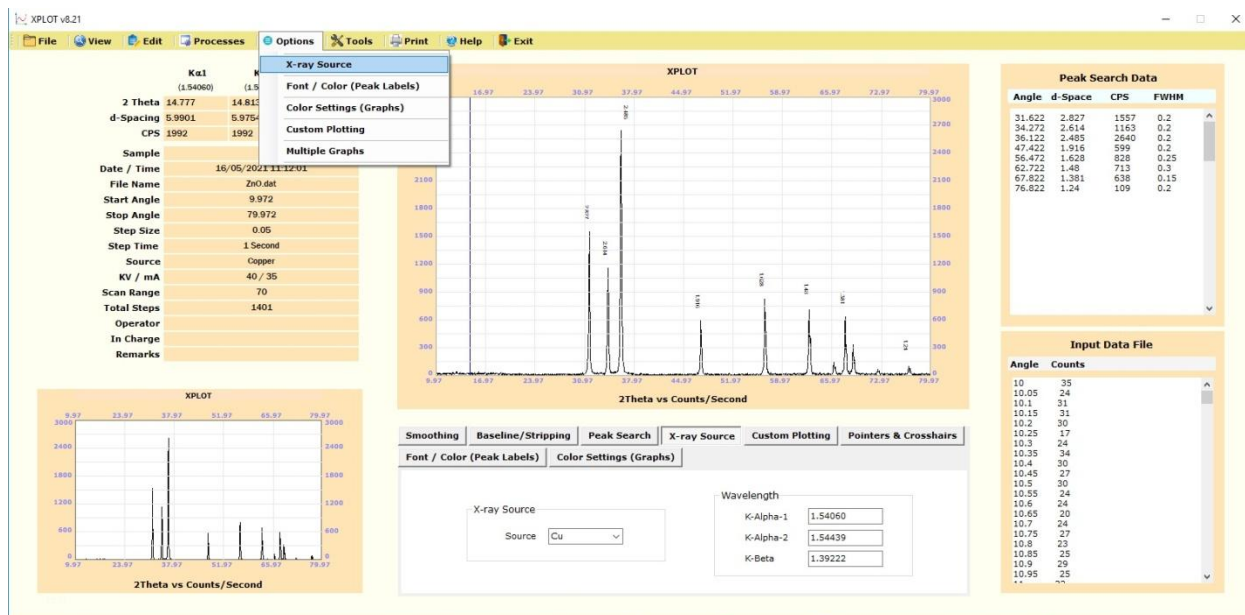
Peak Angle (degree)

Peak Width (degree)

Angle Degree	FWHM Degree	Size um	Av. Size um
31.622	0.2	4.127	4.127
34.272	0.2	4.155	4.141
36.122	0.2	4.176	4.153
47.422	0.2	4.337	4.199
56.472	0.25	3.606	4.08
62.722	0.3	3.1	3.917
67.822	0.15	6.38	4.269
76.822	0.2	5.068	4.369

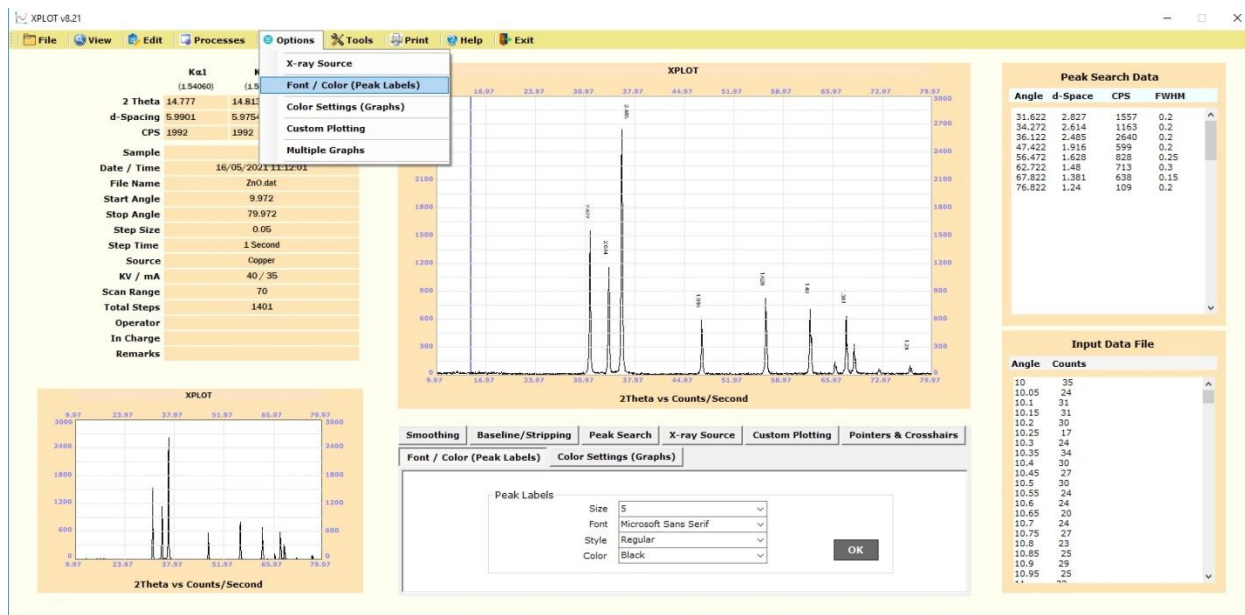
How to Select X-Ray Source

You can select any X-ray source from the list containing Cu, Cr, Fe, Co, Mo and W to use related wavelength according to your input import data. Click on Options TAB → X-Ray Source and the select X-Ray Source in the combo box shown in TAB Control Panel.



How to Change Font and Color of Peak Labels in Main Panel

You can change font size, style and color of peaks labels in Main Panel according to your own choice for your presentation. Click on Options TAB → Font / Color (Peak Labels) and then change font, style and colors of Peak Labels using controls shown in TAB Control Panel.



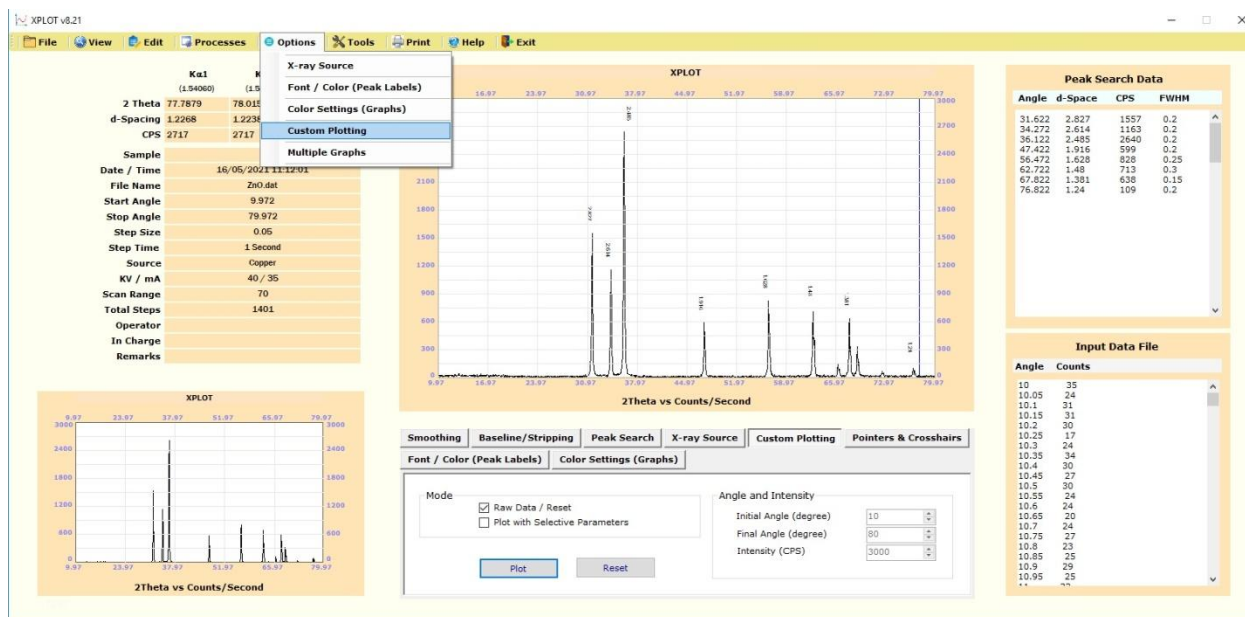
How to Change Color Settings of GUI

You can change colors of different sections of GUI according to your own choice for your presentations. For this purpose click on **Options** TAB → **Color Settings** and then set colors of different sections of GUI using 6 controls shown in Main Panel and Preview Panel of **TAB Control Panel**.



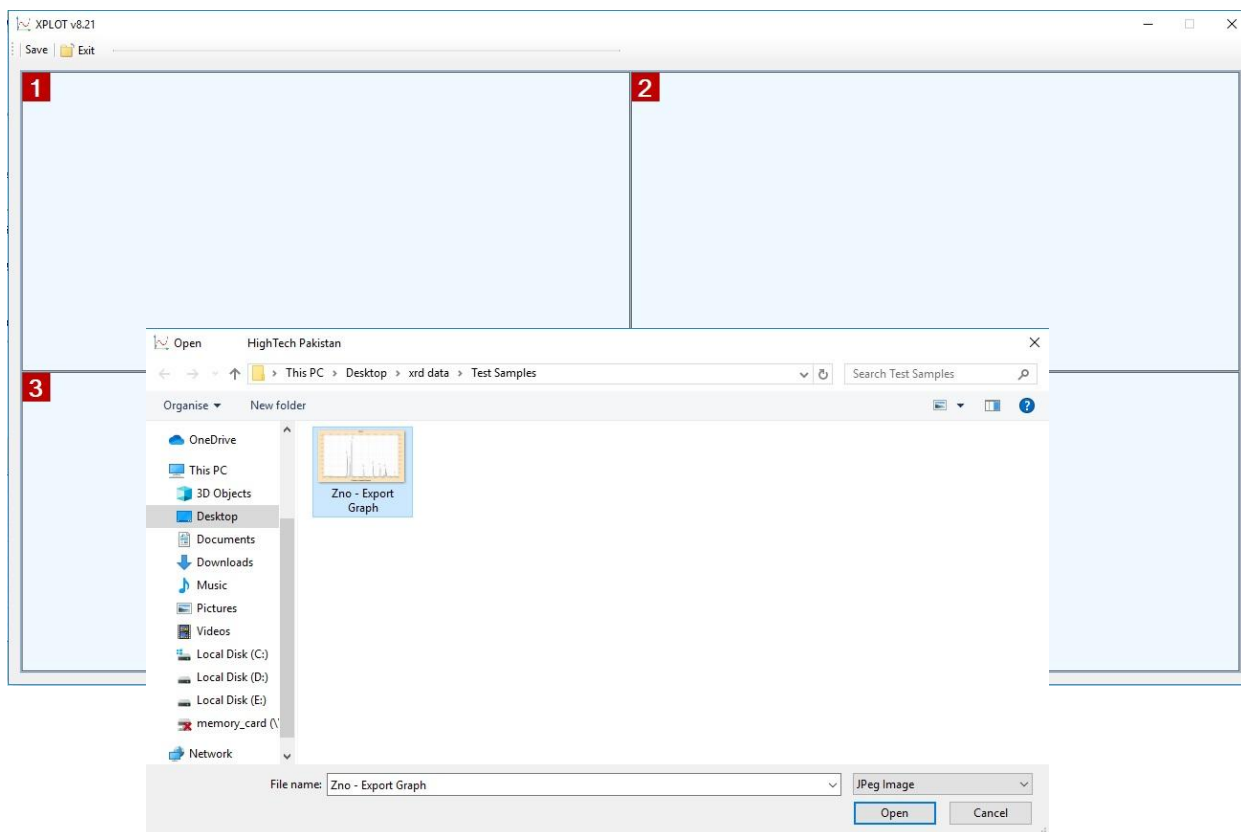
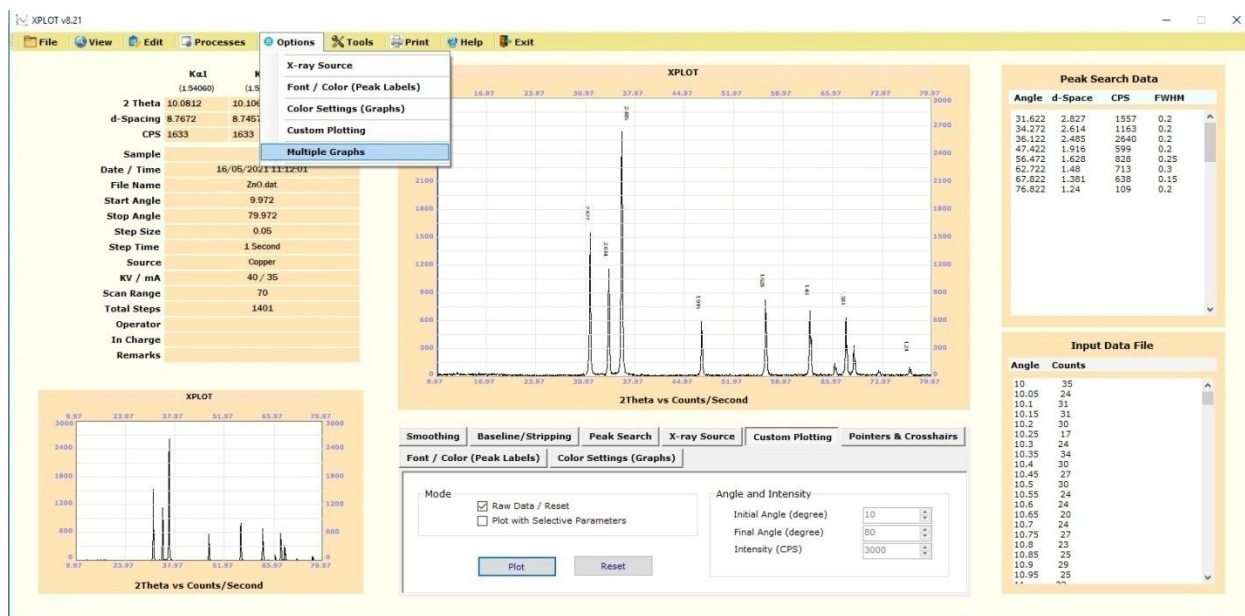
How to Customize XRD Plot

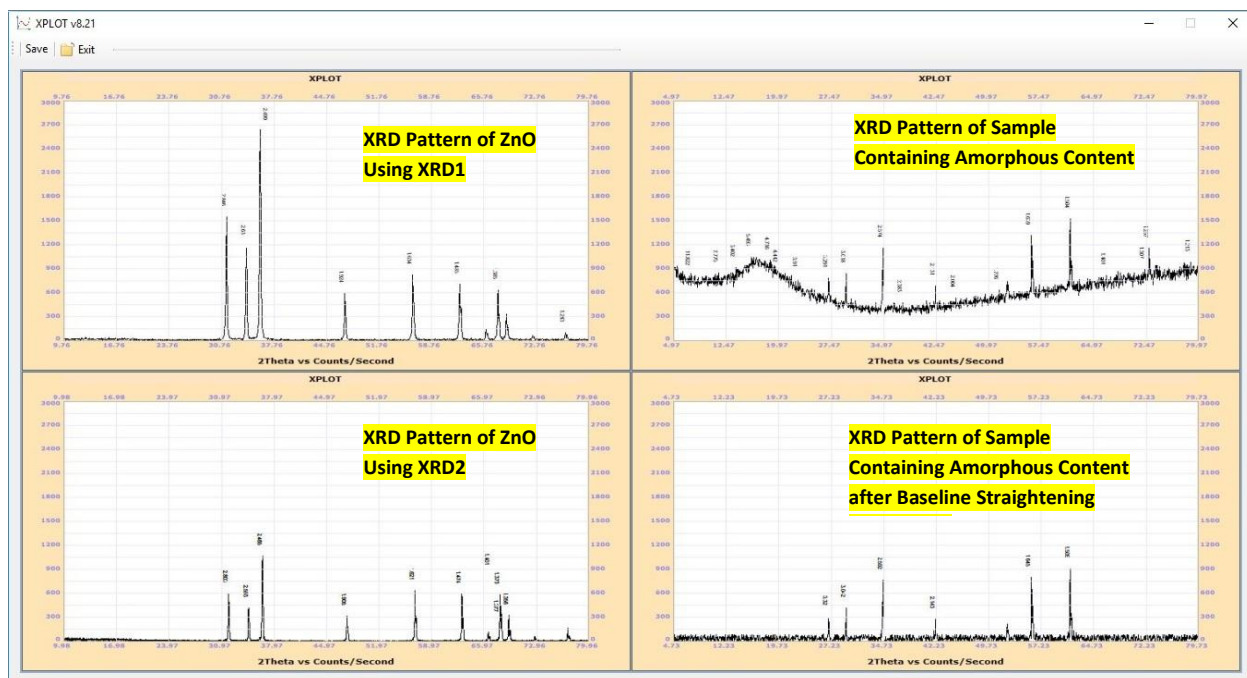
You can modify X-Scale and Y-Scale to get plot of selective range. In this way you can resolve overlapped peaks and use data for other applications. Click on Options TAB → Custom Plotting and then select angle and intensity ranges from the TAB Control Panel.



Display of Multiple Graphs for the Purpose of Data Comparison and other Applications

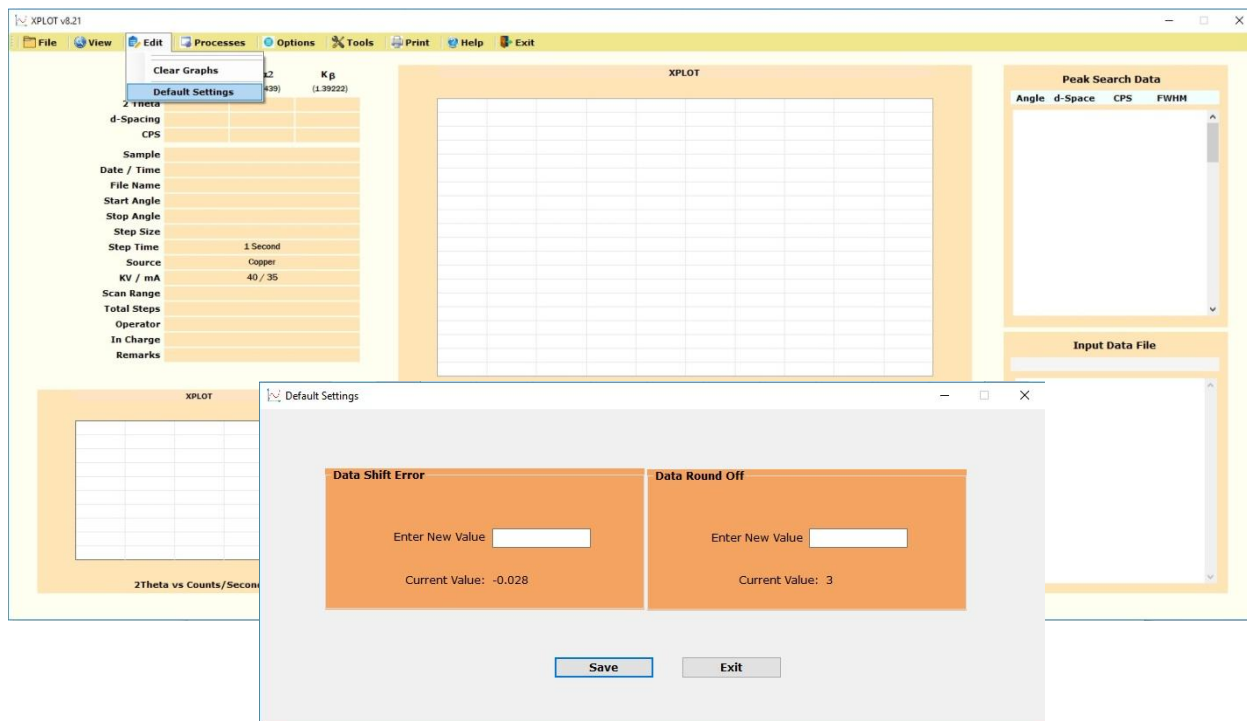
Click on **Options** TAB → clicking on **Multiple Graphs** another form containing 4 rectangles will be shown. By double clicking on any **rectangle 1, 2, 3 or 4** file open dialog will be opened from where you can import image files of diffractions patterns. You can import maximum 4 images to compare and save for other applications and presentations.





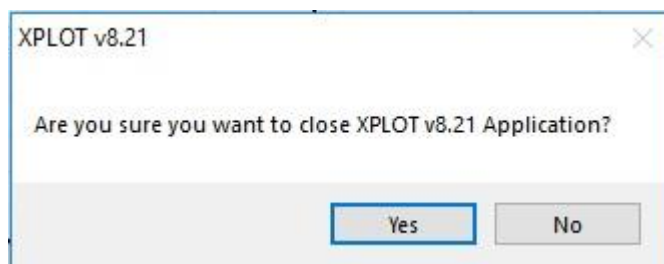
How to Get Corrected Shift in Raw Data

Shift in data is calculated by subtracting the 2 Theta angle of major peak of test sample from the 2 Theta angle of the same major peak Standard sample. This value may be negative or positive. Click on **Edit** TAB → **Default Settings** and then enter the Error Value in the text box. Enter the Error value with negative sign if Error value is negative. Enter the decimal value to round off the raw data.



Shutdown XPLOT

Clicking on Exit on Menu Bar or **File** TAB → **Exit**, Popup window will be display. Click on Yes button if you to shutdown the application or on Cancel button if you still want to continue your work.



Warranty

XPLOT v8.21 is one of the most useful software in the field of X-Ray Diffraction which is used for the processing of raw data. Its Graphic User Interface (GUI) contains all types of controls on single dashboard so its use is very simple. A person having little knowledge of computer can run this software without any hurdle and special training. XPLOT v8.21 contains its license embedded in hardware key which is supplied with the software. Updates are available for life time free of cost. However Hardware key has warranty for the period of one year. In case of damaged or broken hardware key new key will have to be purchased. The duplicate hardware key will be supplied on discounted price which is USD 50. You can run XPLOT v8.21 on any personal computer Windows 7 and above. XPLOT v.21 can be used on that computer which holds hardware key plugged in on its any USB port. Therefore, one can run XPLOT v8.21 on single computer only at a time. To run XPLOT v8.21 on two or more computers one has to purchase duplicate hardware keys. The price of duplicate hardware key is USD 50 and can be purchased by the clients who had already purchased XPLOT v8.21.

For order information, inquires and troubleshoots please visit www.hightechpakistan.com to find our contact details and address.

Thank you