# Program PLATE – Getting Started

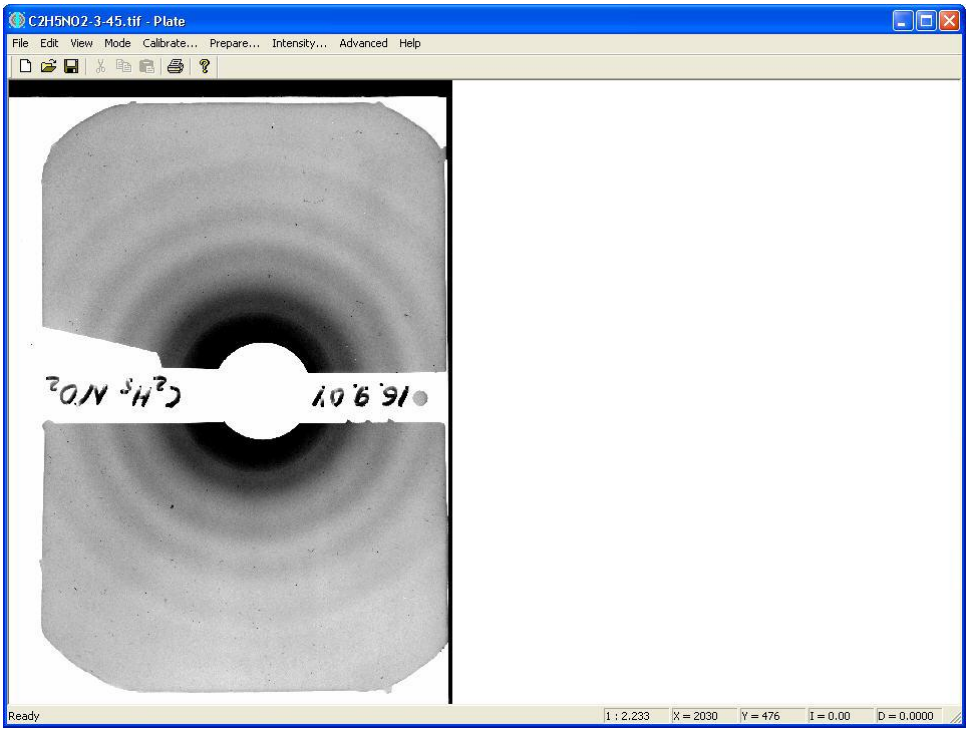
I.V. Kochikov, D.M. Kovtun, Y.I. Tarasov.
A new software for processing the radial symmetric diffractograms.
Numerical methods and programming. Section 2, Programming. 2008. V. 9**.** p. 12–18.
http://num-meth.srcc.msu.su/english/index.html

**1. Start PLATE application by double-clicking the icon.**

Warning: if you plan to automatically determine wavelength using gas standards (e.g. CCl4 or benzene), make sure that directory where Plate.exe libes contains also appropriate .edm files.

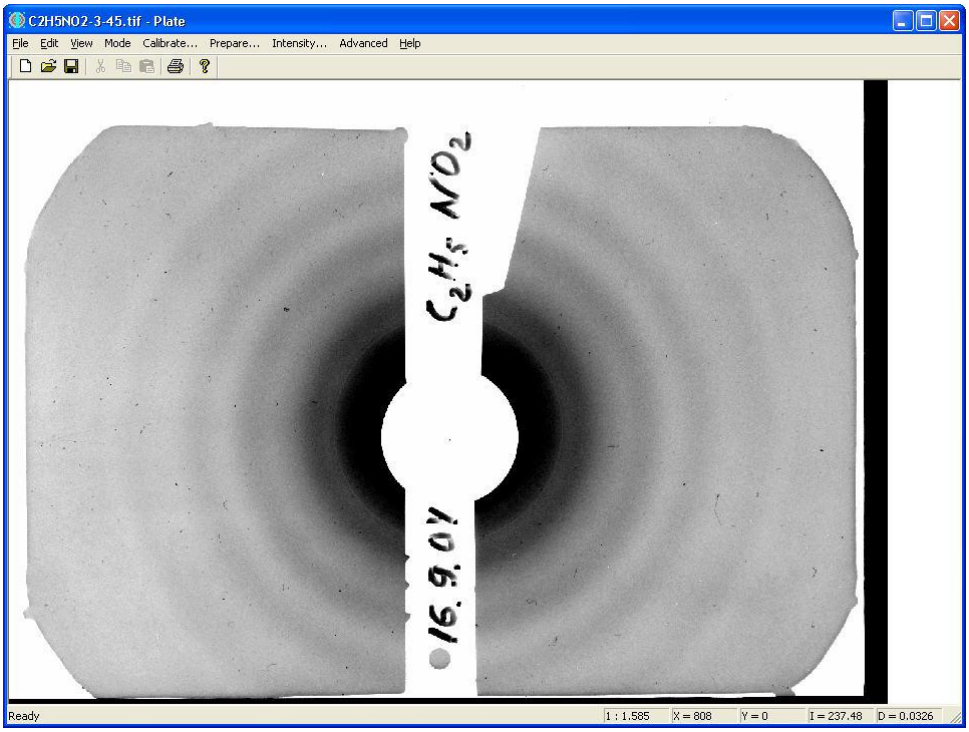
**2. Load image file.**

Run menu command **File/Open**. At present, Plate works with BMP and TIFF files; it is strongly recommended that you use 16-bit TIFF files; however, 8-bit may also be fine. If you have other input format for the scanned images, please convert them to TIFF using any available graphic editor.



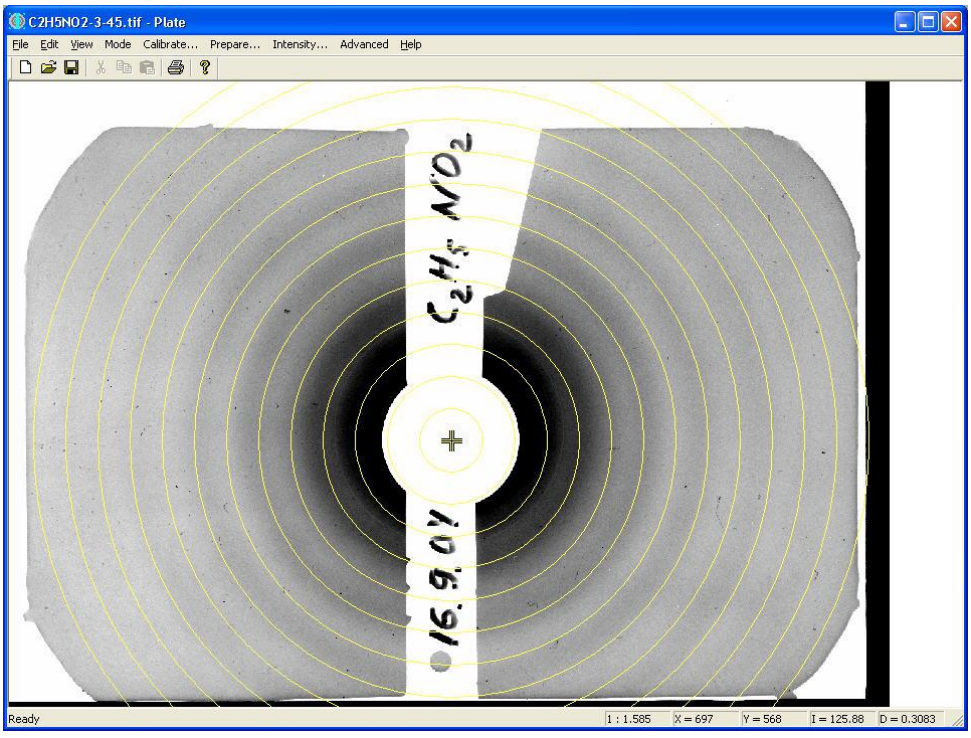

You should see the picture immediately (this picture shows you an example).

For further processing, it is recommended that the longer side of your image is positioned horizontally. If it has been scanned differently, use menu option **Edit** where you can choose appropriate rotation of the image. The following picture shows initial image after the command "**Right 90**".




### 3. Set approximate center of the diffraction pattern.

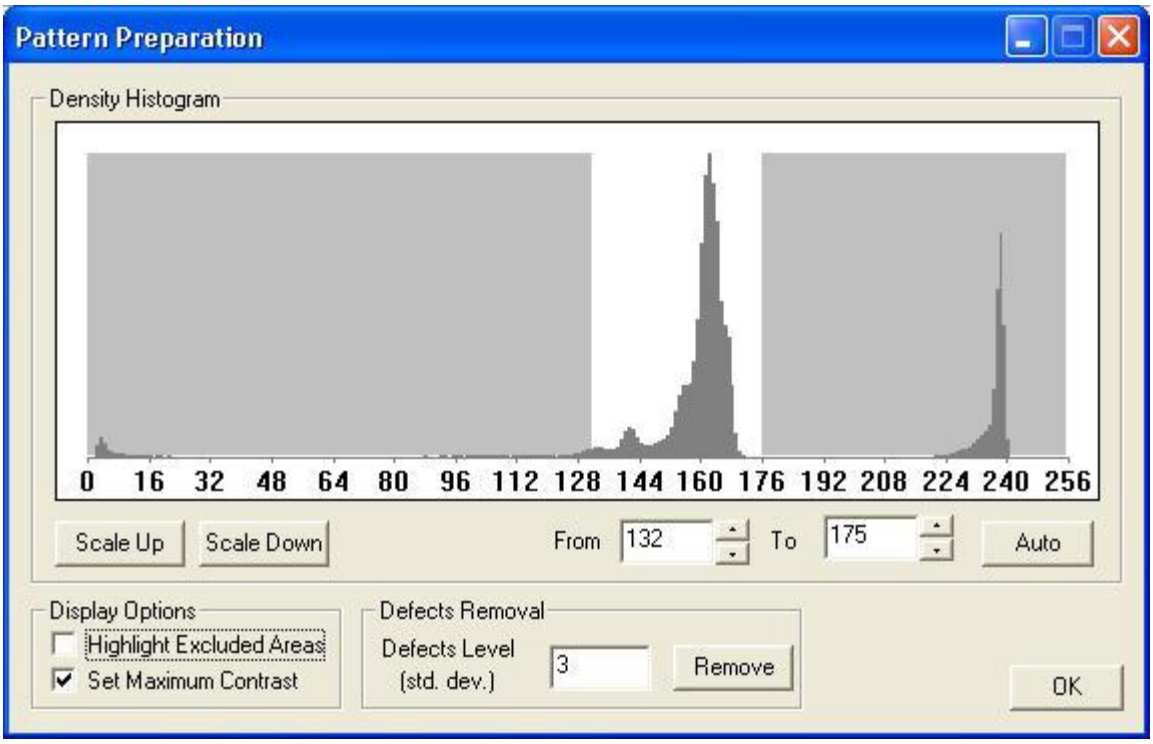
Click left mouse button somewhere near the approximate location of the diffraction pattern center. You will see yellow concentric circles that help you to adjust center position; use keyboard arrows to adjust position of the center.



This action may also be done after the next.

**4. Adjust display to the actual plate density settings.**

Depending on the substance and scanning options, the image that you see may lack contrast. **Note that PLATE is showing you an already contrasted image**. It is convenient to adjust display and processing settings to the optical density of the pattern. To this purpose, choose menu item **Prepare…**

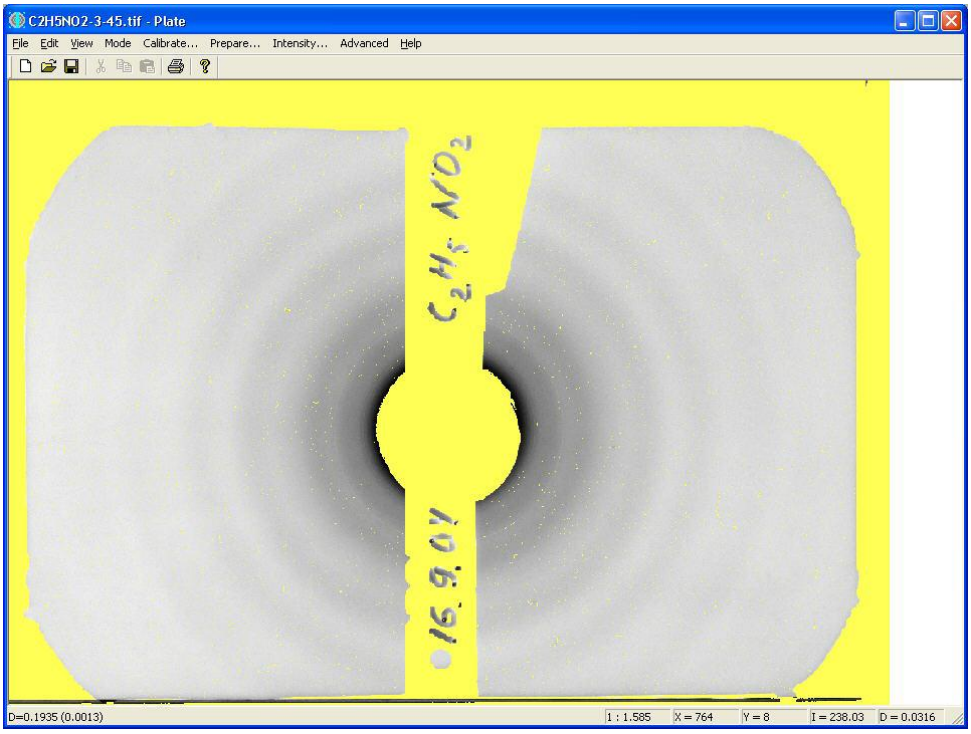



In the dialog that appears, you can see a histogram of the whole pattern (value 0 corresponds to black – that is, completely opaque, and 256 is white – that is, completely transparent). A white strip between the values "From" and "To" shows that range of densities that will actually be processed by the program; all the rest will be excluded. To see what pixels are actually excluded from the processing, check "**Highlight Excluded Area**" box. All excluded areas will be marked yellow.

Using "**From-To**" settings, make sure that all parts of the picture that you want to be processed are not painted yellow. "**Defects Removal**" option will remove all pixels that have densities different from the neighbors by more than "Defects level" measured in standard deviation units. Click "**Remove**" button once you have adjusted From/To levels.

The checkbox "**Set Maximum Contrast**" allows (when unchecked) to see the original state of the image, without any contrasting.

At the next picture, you can see the result of "Prepare" procedure. Before exiting "Prepare" dialog you may want to disable highlighting excluded areas; highlighting does not affect further processing. This can also be done later.




**5. Scrolling and zooming.**

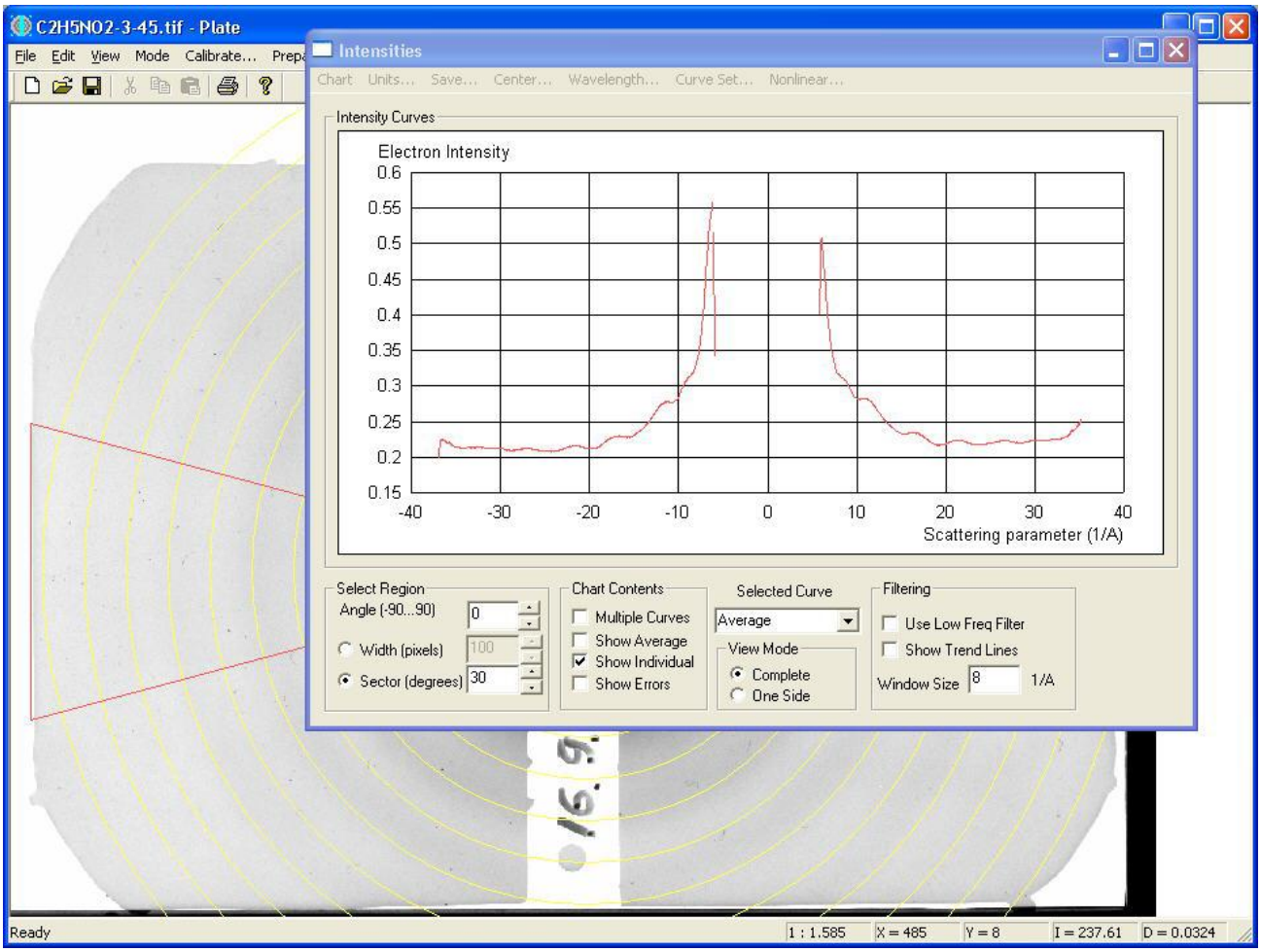
You can change display scale using menu command **View** (Zoom In and Zoom Out). **Zoom Auto** will fit the image to the window; **Zoom 1:1** will show the picture with its original size. Use right and bottom sliders to navigate through the image when its size is larger than the size of the window.

As you move the mouse over the image, in the status line at the bottom you see the mouse cursor coordinates (X and Y), image file values I (in the range 0-255), and optical densities (D).

**Warning**: if you have not loaded calibration file for your scanning device, the values of displayed optical densities cannot be reliable. They are calculated using the simple formula ln(256/I), and may depend on the scanner settings and many other details. For accurate data acquisition, you will need to calibrate your device. See the chapter **Scanner Calibration** for more detail.

**5. Generate intensity curves.**

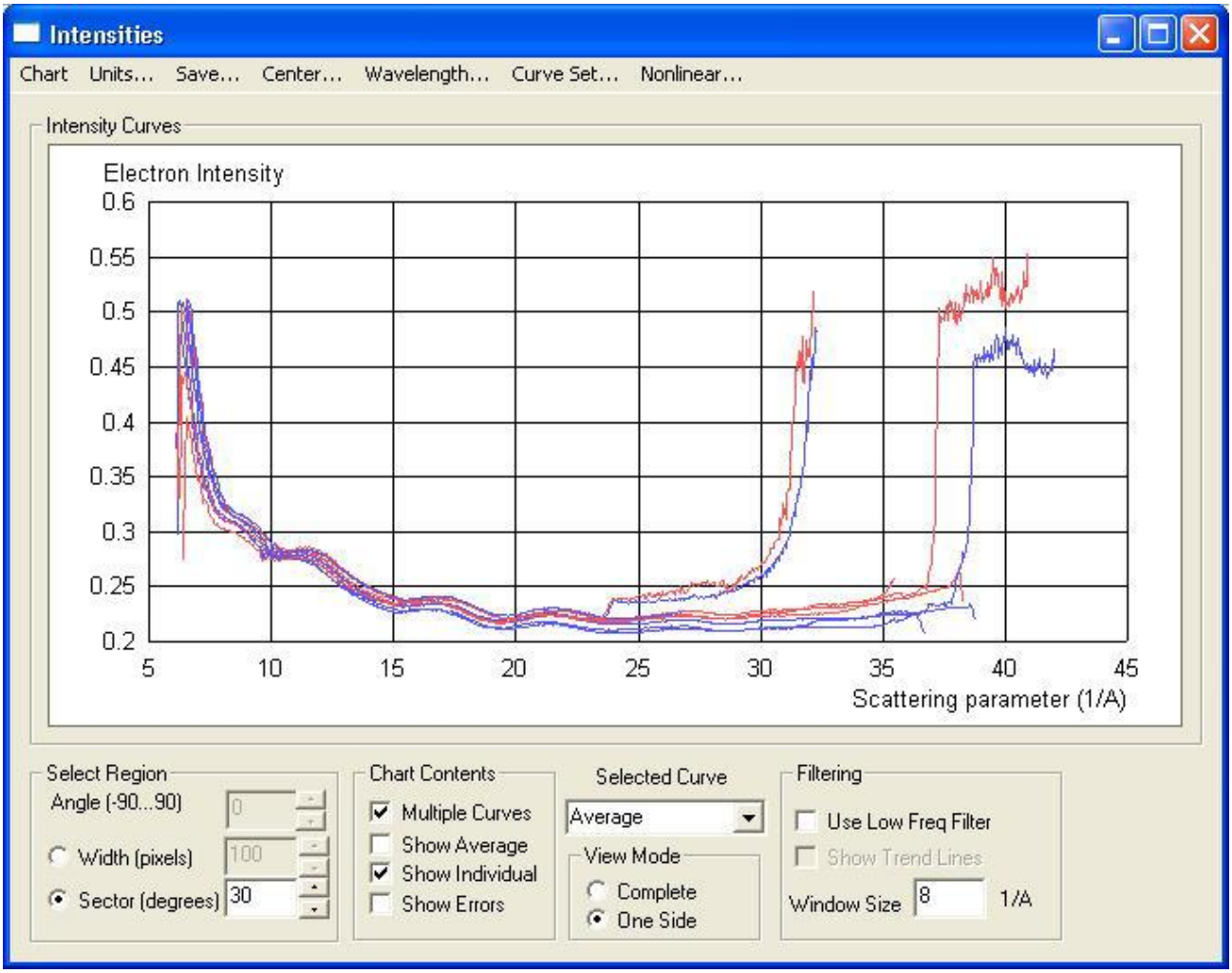
Choose "**Intensity…**" menu item. The following window will appear.




In the plot area, you can see the intensity profile through the whole plate. This profile is obtained by measuring intensities at every pixel of the image and then averaging it. The averaging is always done over the arcs of concentric circles; averaging area may be a strip or a sector. In the picture, choosing button "**Width (pixels)**" will mean averaging over a strip with a specified width (in image pixels). Choosing "**Sector (degrees)**" will average over a sector with a specified angular width (in degrees). Averaging area is shown in the background picture with red (in this particular case, it is a sector 30 degrees wide). The value "**Angle (-90…90)**" shows a strip or sector orientation; 0 degrees corresponds to the horizontal position of the data acquisition area. Change these values to see what is the effect on the curve; look also at the red boundary in the background image.

We recommend to use sector area to suppress noise errors at large radii where the signal is usually weak. Sector width is chosen based on the particular properties of the plate being analyzed.

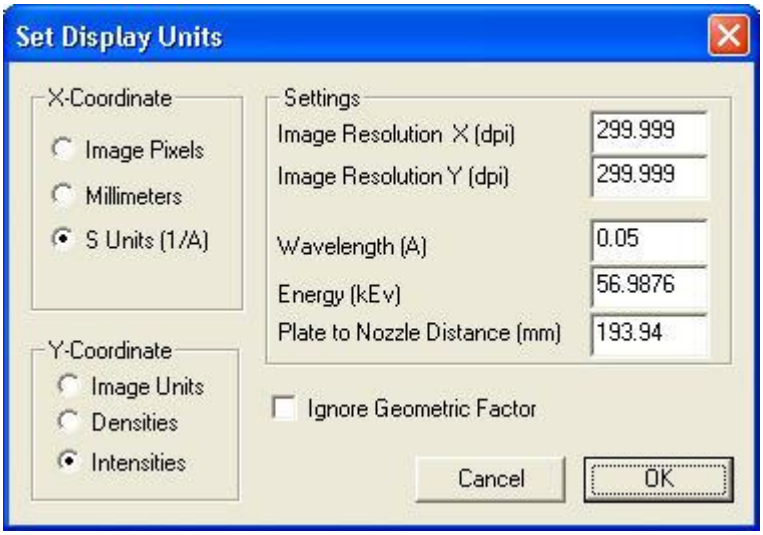
**View Mode** control allows you to see one-sided pictures – in this case, intensity curves are drawn from the center to peripheral areas of the plate (left side is drawn in blue, and right side in red). **Multiple Curves** checkbox shows simultaneously the curves calculated for the different orientation of the processed area (strip or sector).




In this picture, you can see the curves taken for sector orientations of 0, ±30 and ±60 degrees (two curves for each of 5 orientations).

You can choose any fragment of the picture for closer inspection; to this purpose just draw a rectangle in the picture (choose left-top corner, press mouse button; drag mouse to the bottom-right corner and release mouse button). If you decide to restore initial state of the picture, use menu item **Chart/Zoom Auto**.

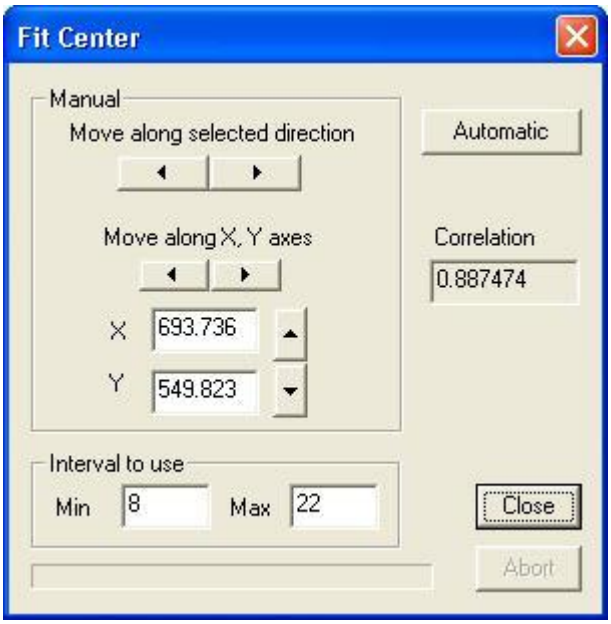
Before proceeding any further, some necessary values should be set. Intensity window may display the resulting values in the units of optical density, electron intensity or scanner measurements; arguments axis may be shown in image pixels, distance units or scattering parameters. Proper settings are set using window menu item "**Units…**"




In this dialog, wavelength or electron energy may be set; once one of them is defined, another is recalculated. Plate-to-nozzle distance is obviously necessary, as well as image resolution which is measured in pixels per inch (25.4 mm). Other options shown here will be discussed later.

**6. Accurate definition of the diffraction center position.**

Choose menu option **Center…** The following dialog will appear on the screen.

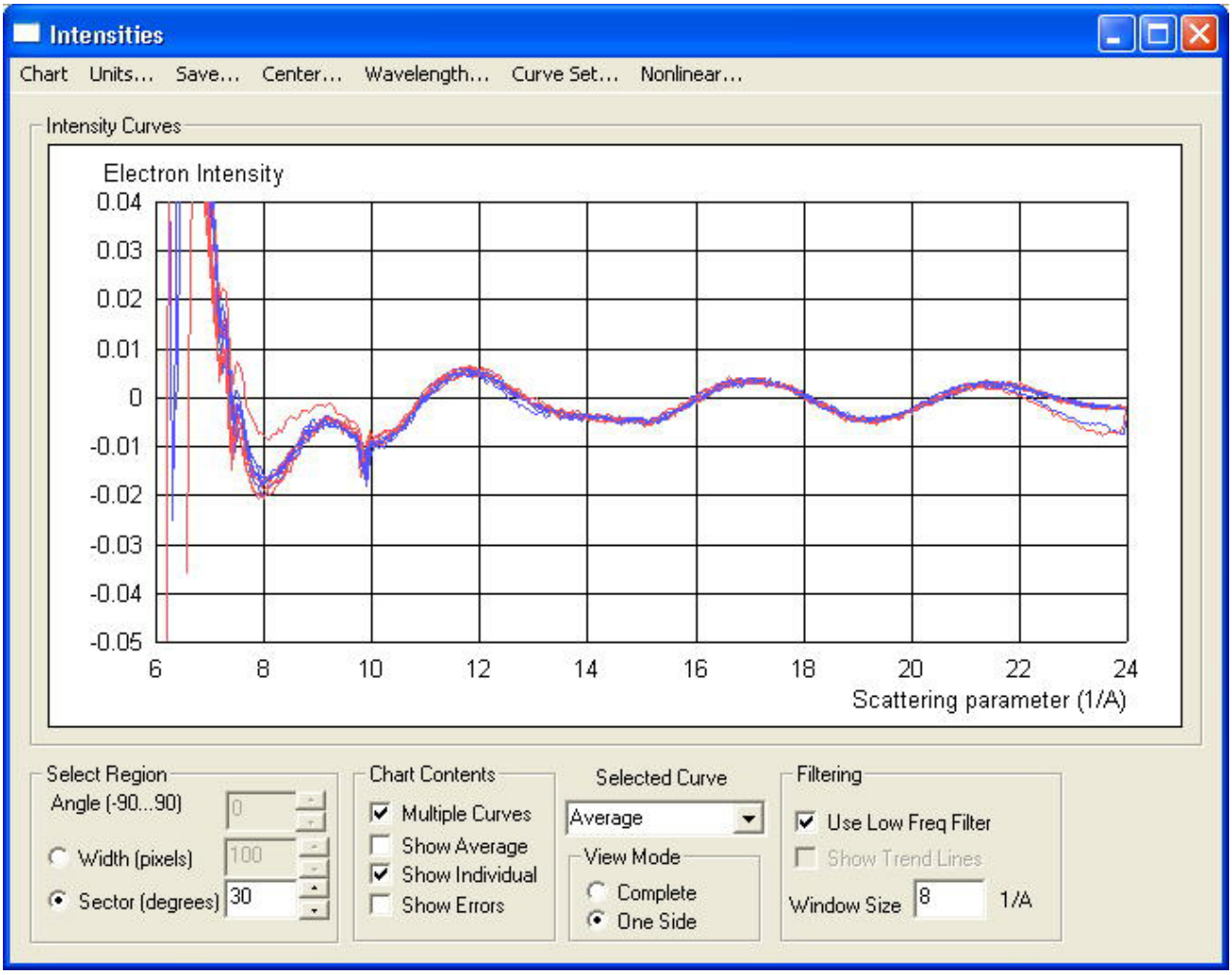



The procedure of adjusting the center uses 10 curves taken at different orientations on the plate, It removes low-frequency contents of each curve and tries to adjust center position so as to maximize correlation between the curves. You can modify the center position manually (using arrow buttons near X, Y edit boxes, or change the contents of edit buttons, trying to maximize the value in "**Correlation**" box, or just manually inspecting the resulting intensity curves. A recommended alternative is to run an automated procedure by pressing the button "**Automatic**".

It is important to set a reasonable interval of arguments: it is desirable that all (or most) curves should be properly acquired in this interval.

Once the center is defined, you can close the dialog; the setting will be saved and used in further actions.

The following picture illustrates the quality of center fitting.




In this case, the intensities are displayed with low-frequency content filtered out (see the checkbox "**Use Low Freq Filter**"). Note an image defect near s = 10; in this experiment, a sector had a defect that resulted in concentric ring on a plate. Generally, all 10 curves are indistinguishable within the random error range.

**Important note**: before starting :Fit Center" dialog, it is strongly recommended to set the option "**One Side**" in the Intensities window, and enable "**Use Low Freq Filter**" checkbox. These settings improve the accuracy of center determination.

## 7. Saving an intensity curve

For saving a curve, choose menu option **Save** in Intensity window. You will be prompted for an interval in which data should be saved ($s_{min}$, $s_{max}$) , and a step $\Delta s$.

A curve to be saved is obtained by averaging the initial curve through $\Delta s$ intervals. Output looks like follows:

```
****** Plate 1.0 Scanned image processing results *******

===  Input data ===
Input file name:       D:\Chemistry\Fon\Images\04.sep.16_nitroetan\C2H5NO2-3-45.tif
Calibration file name: Unknown.clb
===  Preprocessing ===
Valid scanner intensity range: From 90 to 175
Noise points suppressed at level 3.000 sigma
===  Scaling ===
Wavelength = 0.050000 Angstrom
Plate to nozzle distance = 193.940 mm
===  Adjustment ===
Picture center detected at (693.736 549.823) pixels
===  Used Area ===
  Sector(s) 90 degrees wide
===  Averaging ===
Left and right curves averaged

sMin= 7.000
sMax=30.000
sStep= 0.200
  0.402224  0.372702  0.352073  0.342116  0.328196  0.320344  0.316413  0.313334
  0.311412  0.309373  0.306141  0.302721  0.297736  0.292528  0.285025  0.283184
  0.281248  0.279646  0.279142  0.279668  0.280317  0.280316  0.279602  0.278296
  0.276608  0.273944  0.270407  0.266818  0.263056  0.259319  0.255367  0.252201
  0.248984  0.246458  0.244115  0.241876  0.240036  0.238021  0.236014  0.234552
  0.233213  0.231963  0.231673  0.232024  0.232416  0.232998  0.233322  0.233875
  0.233943  0.233665  0.233438  0.232402  0.231362  0.230012  0.228147  0.226324
  0.224259  0.222450  0.220675  0.219032  0.217862  0.217092  0.216645  0.216941
  0.217305  0.217913  0.218959  0.219925  0.221013  0.222042  0.222909  0.223126
  0.223408  0.223384  0.223036  0.222444  0.221661  0.220759  0.219935  0.218944
  0.218264  0.217504  0.216958  0.216535  0.216485  0.216297  0.216471  0.216851
  0.217094  0.217555  0.217905  0.218204  0.218721  0.219223  0.219807  0.220219
  0.220726  0.221071  0.221315  0.221606  0.221639  0.221297  0.220982  0.220254
  0.219697  0.218957  0.218348  0.218103  0.217993  0.218166  0.218530  0.219154
  0.219852  0.220621  0.220892  0.221054

 7.000    0.402224       0.000648
 7.200    0.372702       0.000518
 7.400    0.352073       0.000442
 7.600    0.342116       0.000407
 7.800    0.328196       0.000363
 8.000    0.320344       0.000305
 8.200    0.316413       0.000265
```

(the rest of file is skipped).
The data is represented in two formats; the first is an array of intensities, while the second is a set of three columns: an argument (s), measured intensity and its standard deviation. Standard deviation is obtained during averaging procedure.

**Important note**: before saving intensity curve, make sure that "**Use Low Freq Filter**" box is unchecked.

## 8. Automatic determination of the wavelength.

In a usual procedure of electron diffraction analysis, a standard substance (like CCl4 or benzene) is registered to determine the wavelength of electrons. “Plate” allows automatic determination of the wavelength for some of the substances.

The only options that you have is opening the dialog using **Wavelength** menu command. Then a standard should be chosen. It is important to set proper range for the minimum and maximim limits of scattering parameters. The final result is obtained after pressing the button “Fit Wavelength”. The value of wavelength is automatically transferred to the rest of the program. All further actions with this and other images will take place with this wavelength.

## 9. Calibration of scanner characteristics.

This is done using some standard photographic gray scale. Since the procedure is so far not quite automated, it is recommended to use pre-defined calibration files which should have the following contents (here is an example):

```
Calibration Curve created on Mon Jan 08 15:15:59 2007

Density     Image Value
     0.000         221.97
     0.250         145.13
     0.500          98.19
     0.750          67.71
     1.000          47.76
     1.250          32.48
     1.500          20.95
     1.750          14.37
     2.000           9.81
     2.250           6.49
     2.500           4.24
     2.750           2.94
     3.000           1.92
```

The first three lines of the file should be ignored, while the rest contain densities and scanner values (0…256). The file should have extension “.clb”; an example of such file is enclosed with the program.

## 10. Saving configuration data

Once you have loaded the image and made some adjustments (like setting intensity range, rotating image, determining the center, wavelength, or setting plate-to-nozzle distance, etc.) all this data is stored in a special configuration file that has the same name as image file and extension “.inf”

When you load the same image for the second time, you will be prompted to apply all the actions that you have previously done to this image. Pressing “OK” ensures that you have all valid parameters loaded, and may directly proceed with extracting intensities.