

The HSvu app.(HighScore view application) displays all kinds of X-ray diffraction scans in various file formats.

Additionally it shows and reports all details from an X-ray powder diffraction analysis performed by the <u>HighScore analysis software</u> from <u>PANalytical</u> (documents in the proprietary .HPF format). <u>HighScore Plus</u> (HighScore with the Plus option) is suported too.

More explanations are found at:

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You can also download the complete explanations in PDF format with bookmarks as <u>HSvu.PDF</u>.

By downloading and using the HSvu application you agree to the terms and conditions. The smallprinst (the actual end-user-license-agreements) are here:

EULA for the HSvu App on MAC and iOS devices EULA for the HSvu App on Android devices

ATTENTION:

HSvu requires processing power and some memory. The data file size handled by HSvu is limited by the device capabilities and its performance.

HSvu Introduction



Experience the power and ease-of-use of HighScore and HighScore Plus with the HSvu app.:

- Use six different graphical views for references, single and multiple scans, quantifications and 3dimensional graphs
- Pinch-zoom for details like you do with HighScore
- Get a complete overview on measurement conditions, scans, peaks, profiles and crystal structure data
- See how identified reference patterns fit to the measurement and what are their quantities.
- Switch easily between graphics and textual information (= reports)

- Unravel the parameters used in a diffraction analysis and its history
- Export bitmaps or reports covering either pieces or of the complete diffraction document

The actual version 1.0.12 is another bugfix and enhancement on the initial release version 1.0 with the following changes:

- General improvements
- Updating the HighScore (Plus) document format to version 5.2, released in February 2023
- Displays and reports the complete .XRDML scan data, as now included in every new (v.5.2 or higher) HighScore document (in .HPF2 format).
- Display and report of PDF (= atomic pair distribution function) simulations and fits.

▲ **ATTENTION:** HSvu is a display or viewing application.

It shows existing data, but it neither performs an analysis nor does it change data or converts file formats.

Import of scans or documents from email:

You can directly open the selected email attachments in HSvu:



Import of scans or documents from drop box:

Select the scan or document on go to Open with..., then go to HSvu.



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The following file formats are supported in HSvu:

- PANalytical: .HPF and .HPF2 (proprietary HighScore document)
- PANalytical: scans .XRDML
- PANalytical: .2Dint (ASCII format integrated from a 2D area detector)
- ASD Inc.: .ASD (binary NIR spectrum)
- Philips: binary scans .RD, .SD, .FP, ASCCI scans .UDF, .LIS
- Bruker: binary scans .RAW versions 1, 2, 3 and 4, ASCII scans .LST, .UXD, .XDD
- Crystallographic information file .CIF (scans only!)
- General ASCII scans X-Y(-Z) table .ASC
- DBW-Rietveld: ASCII scans .RFL
- GSAS: ASCII scans .RAW, .XRA
- ICDD: PD3 ASCII scan .PD3
- JCAMP: ASCII scans .JDX or .JCP
- LH-Rietveld: ASCII scans .LHP
- MDI: ASCII scans .MDI
- Rigaku: ASCII scans .ASC, .FI, .RAS, binary scans .RAW
- Scintag: binary scans .RAW
- Seifert: ASCII scans .ASC
- Shimadzu: binary scans .RAW
- Skrowonek: ASCII scans .UDS
- Stoe: CSD-PROFAN ASCII scans .PRO, .DAT, binary scans .RAW

• Thermo Scientifique: scans .XML

🐺 Tip:

To compare several scans with each other, insert them into a document in HSvu.

HSvu User Interface

Depending on the available size and resolution, the graphical user interface is shown in different ways. The major interface elements are:



1. Files List:

The list of .HPF documents and data files available for HSvu. At the top there are some example files from *PANalytical*, which you cannot delete. The user files are situated below the examples.

2. QUnzoom (double-tap): Zoom-out after you zoomed into the graphics display; double-tap is an alternative way to zoom in or out.

- ¹ Share selected file: Send the selected file from the file list to somebody else.
- 4. ¹ Share HSvu data: Share data shown in HSvu with your friends. Graphics can be printed, emailed (iMessage) or stored (iCloud);
 Peports can be emailed (zipped report file plus)

Reports can be emailed (zipped report file plus style sheet plus graphics).

5. Main graphics / text area:

The main area displays graphical or textual information about a document or scan data. The actual graphics view is selected under <u>HSvu</u> <u>Settings</u>. Graphics is often shown on two panes. The (mostly) textual information is selected under <u>HSvu Reports</u>.

5a. Y-axis area:

Double tap to directly change the Y-axis scaling.

5b. X-axis area:

Double tap to directly change the X-axis scaling.

6. Opening mode:

Switch between opening a data file or inserting a data file into a document.

▲ **ATTENTION:** You cannot insert a document into another document. Insertion works only for scan files.

7. Tab bar below the graphics switches between:

- 🛱 Graphics,
- 🛱 Settings,
- 🛱 Reports, or a
- Pie chart.

Note:

The availability of certain graphics or reports is depending on the actual data present (or not!) in the selected .HPF document or in the selected scan.

The graphics always show scan data. From a HighScore document more data like peaks, reference patterns, a profile, a difference plot and more are shown.

Most graphics cover two panes, the main graphics above and the additional graphics pane below.

You change the graphics displays (both panes independently) with the <u>HSvu settings</u>.

Tip: Some graphic properties are unavailable in HSvu. For completely customized graphics proceed as follows:

- 1. Set all graphic properties according to your needs in a document using the original HighScore software.
- 2. Save this document from HighScore.
- 3. Open the document with HSvu.
- 4. Save the current graphics settings to the HSvu template.

Reports are the way to look at different information in a HighScore analysis document or from a scan file. Reports contain textual information and sometimes graphics as well.

In HSvu, reports replace the detailed lists with textual information present in the original HighScore software.

Select one of the predefined reports:

- All document properties: Shows meta information about a HighScore document including contents, statistics, history and the process log with the used parameters.
- All measurement parameters: Shows meta information about a scan.

▲ **ATTENTION:** This information depends strongly on the scan format and its header! Missing essential information about a scan (used wavelength, scan axis, ...) is supplied by a predefined instrument default - exactly as in the original HighScore software.

In contrast to the original HighScore software you cannot change the instrument default in HSvu.

• All structure data: Complete, detailed structure data report including distances, angles and positions of atoms.

- Anchor scan: Shows all data points with position intensity and, if present, ESD's (Estimated Standard Deviation values) from the anchor scan.
- Crystallographic peaks: Shows crystallographic peak details like hkl triplets, multiplicity, Fobs and Fcalc...
- Fancy: Shows an example of a complex report with several sections in it.
- Matched peaks: Shows the peaks found and the matching reference pattern(s) after a phase identification.
- Pattern list: Shows all identified (= accepted) reference patterns after a phase identification in a HighScore document.
- Original XRDML: Shows the scan data and all instrument settings in unformatted XRDML format.
- Peak list: Shows the most common peak details from the peak list.
- Quantitative: Shows the quantitative results including errors of the quantification, when present. This report shows two quantitative results views, namely the pie chart and the bar graph, plus a table of all numerical results and the numerical result from the anchor scan.
- Scan list: Shows all scans (= data sets) present in a HighScore document.
- Size-strain peaks: Shows peak details like integral width, GAUSS, LORENTZ and structural broadening, crystallite size and microstrain values.
- Structures: Condensed structure data report with important details only.

- XRDML: well-formatted XRDML scan data report.
- PDF: Condensed PDF analysis report with graphics, data lists or (refined) parameters.

ATTENTION:

Some (parts of) reports remain empty, when the corresponding data is absent.

HSvu Quantitative Results

Quantitative results are displayed in HSvu on three tabs in different ways. These results are either based on RIR (Reference Intensity Ratio) values or on (relative or absolute) Rietveld refinements.

▲ **ATTENTION:** The quantitative results tabs remains empty when quantitative data is absent in the viewed HighScore document.

🐺 Tip:

The error of the quantification results is shown in HSvu exactly the same way as it was configured in HighScore for the viewed .HPF document.

Anchor Scan tab:

The anchor scan tab displays the quantitative or layer thickness results from the anchor scan in a pie chart. Numerical results are shown in the legend of the pie chart.

You change the pie chart (from flat to pseudo-3-dimensional) with the <u>HSvu settings</u>.

All Scans tab:

The all scans view shows the quantification in a bar chart for all scans of the document together(MultiQuant view). This is only possible when:

- The number of active phases is the same for all datasets
- The order of active phases is the same for all datasets
- For all datasets there are either RIR-based or Rietveld-based quantitative results available

All Scans Table tab:

The all scans table shows the same information as the all scans tab, but instead of a bar chart it displays all numerical values in a table. You can copy the table and paste it directly into a spreadsheet program, if required.

The columns of this table are shown as they were configured in HighScore for the viewed .HPF document.

The HSvu settings determine how graphics and the pie charts are displayed in HSvu. They also allow access to the About... box, to the website and to this help file. These settings are identical with the corresponding possibilities in the original HighScore software from *PANalytical*.

All scan files are opened with the default view template. You change the default view template by saving your actual settings into the template. All HighScore documents are opened with the view they are saved with. You can change the display in HSvu by changing the settings - but you cannot store the document with the changed display again.

🐺 Tip:

Save any combination of settings you like for future use in the HSvu template file.

About:

Provides a link to the HSvu and to the HighScore websites and to this help system. Additionally shows the release version of HSvu.

View Settings:

View settings change the <u>graphical displays</u>. They are separated into:

Main Views (select):

- Ref. Pattern view
- Analyze view

- Compare view
- 2D view
- 3D view
- Isolines view

Additional Views (select):

- Zoom overview
- Difference plot
- FWHM statistics
- All-in-One (Ref.Patt.)
- Compare mode (Ref.Patt.)
- Separate (Ref.Patt.)
- Ref. pattern view

Axes Settings:

Axes settings change the scales of the X-axis and of the intensity-axis Y:

Y-axis scale (select):

- Linear Y-axis
- Square root Y-axis
- Logarithmic Y-axis

X-axis scale (select):

- *θ* scale
- ° 2 θ scale
- ° 40 scale
- Sin₂ θ scale
- d-spacing [Å] scale
- Arbitrary scale (datasets with different Xaxes)
- Q reciprocal space (for PDF analysis)

or double tap into the axis area to select! Other Settings: This is a mix of settings to change the appearance and the display of graphics, also in combination with zooming.

- Zoom Y-axis too on/off (select please)
- Show scan as line on/off (select please)
- Isolines 3D on/off (select please)
- <u>Pie chart</u> 3D on/off (select please)
- Legend font size (enter please)
- Canvas color (select please)
- Background color (select)
- Export bitmap scale factor (enter)
- Quant. Display (select from: Normal, AsReceived, K-Factor corrected)
- K-Factor (enter)
- File List Mode (select)
- Save current settings to template

All users of HSvu are encouraged to help us improving our software products. Any comment, complaint, question, missing function, bug, cryptic help, wrong result and so on that you send to us is a valuable input for the next version of the software.

It is a good practice to illustrate your comments by sending us a diffraction document (.HPF format), and input data file (various formats) or a screen dump, a report or any other output from the application. This helps to understand your comments and localize possible bugs.

Email is a convenient way sending feedback to us:

- <u>Send us an email</u> by clicking on this link.
- Note: This works only with email software complying with the email standard. Make sure your email software is known to the browser you are using.
- Send an email to: info@malvernpanalytical.com using your usual, non-standard compliant email program.

Please enter the subject: "HSvu v.1.0.12 App. feedback" to ensure a correct routing at our supply center.