What's New

DIFFRAC.EVA V.7.0

Table of Contents

Version 7.0

New Features

Peak Profile Functions

The Pearson-VII and split Pearson-VII functions have been added because they have a better convergence behavior than the Voigt functions in some circumstances.

The formerly available (split) pseudo-Voigt function has been replaced by the (split) Voigt function.

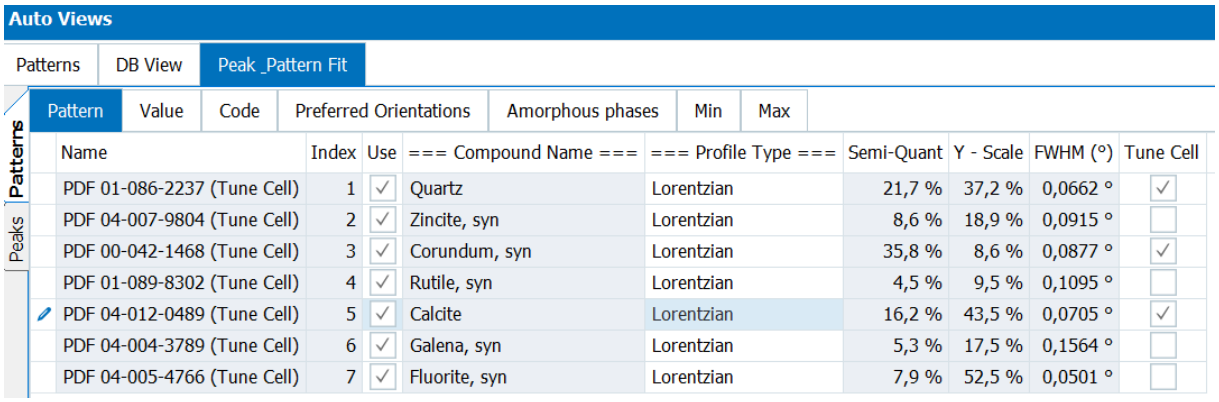
Pattern Fit

The fitting algorithm has been improved and allows refining more pattern parameters:

- Lattice Parameters
- Preferred Orientation
- Amorphous content

Lattice Parameters

The lattice parameter fit is activated with the "Tune Cell" check box in the automatic Pattern table, which is displayed during the fit:

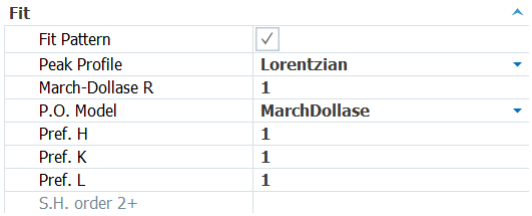


Name	Index	Use	=== Compound Name ===	=== Profile Type ===	Semi-Quant	Y - Scale	FWHM (°)	Tune Cell
PDF 01-086-2237 (Tune Cell)	1	✓	Quartz	Lorentzian	21,7 %	37,2 %	0,0662 °	✓
PDF 04-007-9804 (Tune Cell)	2	✓	Zincite, syn	Lorentzian	8,6 %	18,9 %	0,0915 °	
PDF 00-042-1468 (Tune Cell)	3	✓	Corundum, syn	Lorentzian	35,8 %	8,6 %	0,0877 °	✓
PDF 01-089-8302 (Tune Cell)	4	✓	Rutile, syn	Lorentzian	4,5 %	9,5 %	0,1095 °	
PDF 04-012-0489 (Tune Cell)	5	✓	Calcite	Lorentzian	16,2 %	43,5 %	0,0705 °	✓
PDF 04-004-3789 (Tune Cell)	6	✓	Galena, syn	Lorentzian	5,3 %	17,5 %	0,1564 °	
PDF 04-005-4766 (Tune Cell)	7	✓	Fluorite, syn	Lorentzian	7,9 %	52,5 %	0,0501 °	

Alternatively, the "Tune Cell" pattern property can be used.

Preferred Orientation

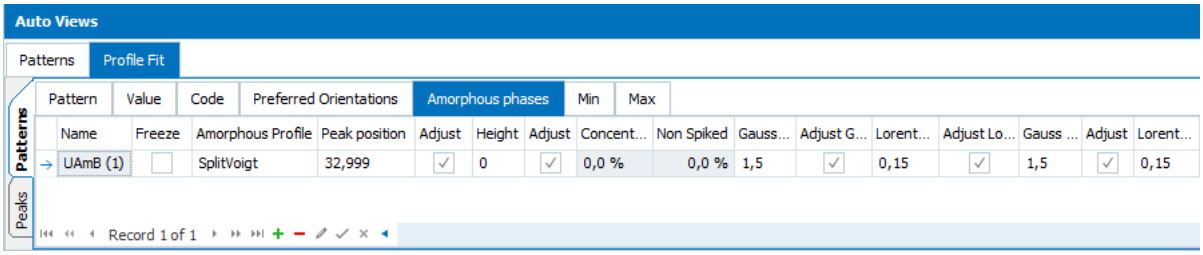
The preferred orientation fit is controlled by new pattern properties:



The March-Dollase model and spherical harmonics up to the 6th degree are available. A Pawley fit without line height constraints is also an option.

Amorphous Content

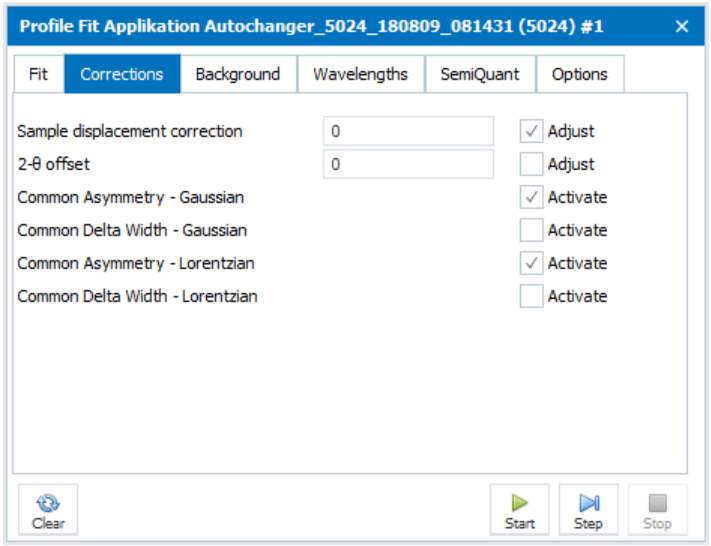
One or more amorphous "phases" can be added on the "Amorphous Phases" tab.



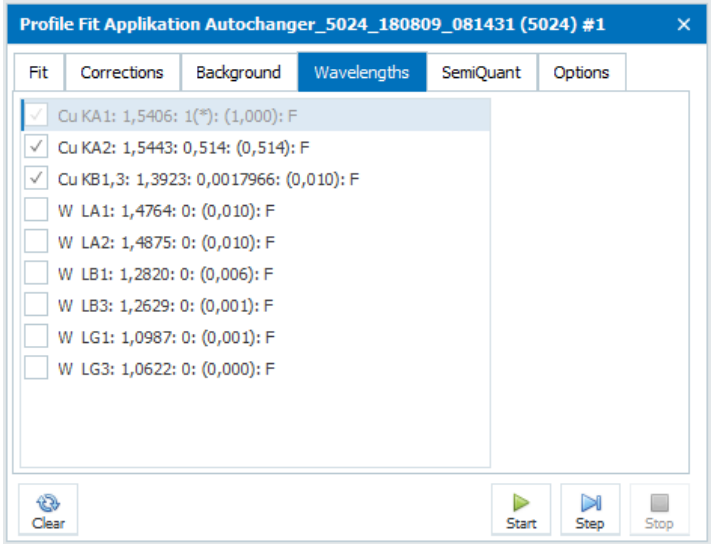
Amorphous entries can be added and removed with the control at the bottom of the Amorphous phases tab:

Profile Fit Tool

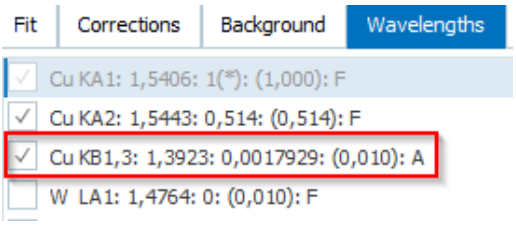
The Profile Fit tool has a new Corrections tab to control various fit parameters:



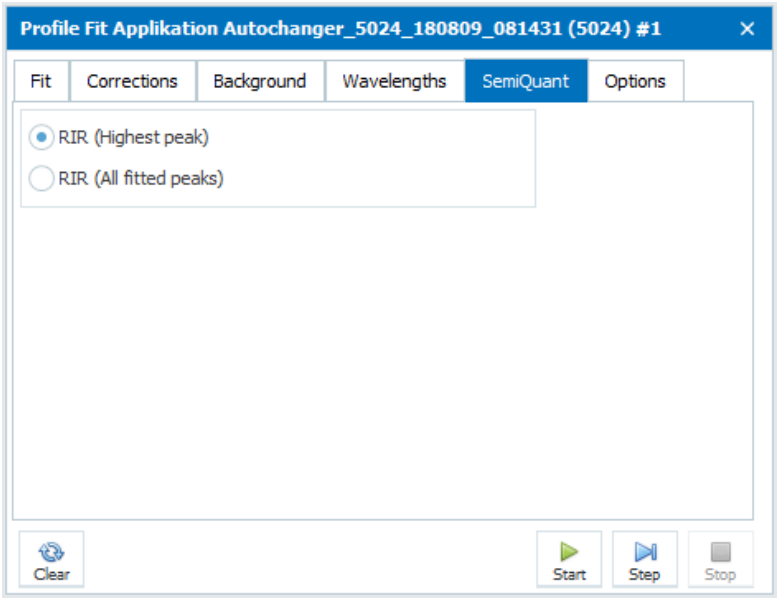
The new Wavelengths tab controls which wavelengths are used in the fit:



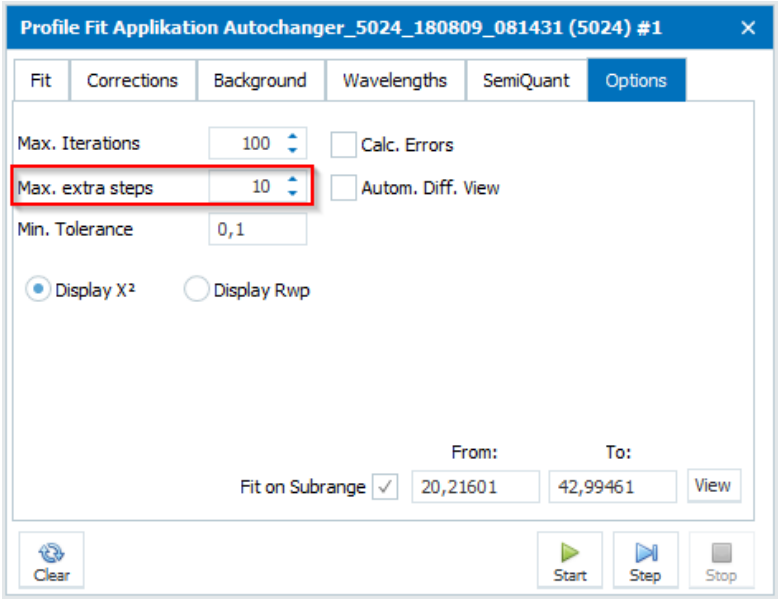
Repeated clicks on a wavelength entry allows switching from a fixed line height ratio to Ka1, marked by an "F", to a refinable ratio, marked by an "A":



Finally, there is a new SemiQuant tab to select how the semiquantitative analysis is carried out:

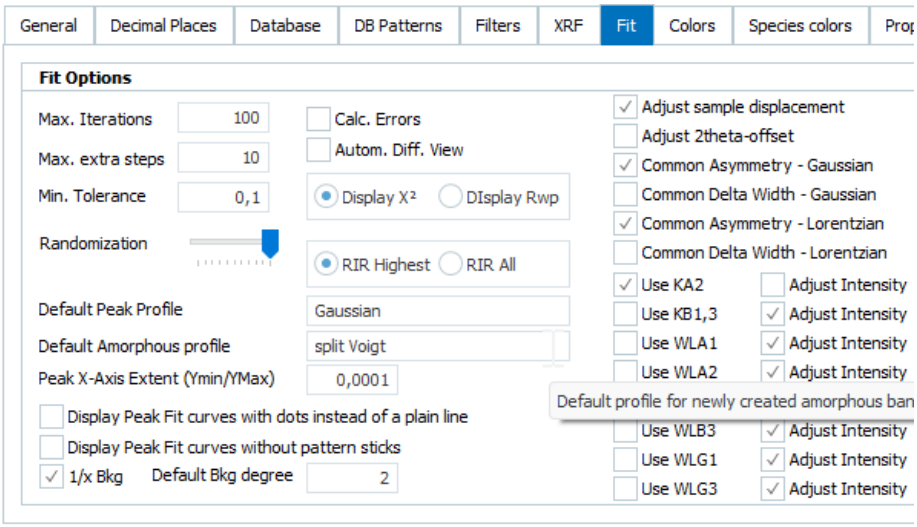


Note: The max. number of iterations on the Options tab (default: 100) is only an approximate value and may be exceeded by some iterations. To limit these extra steps, enter a value. The default is 10:



A "Clear" button at the bottom left allows a reset of the fit results in case of error.

The Settings Dialog's Fit tab was extended to accommodate the new profile fit features:



Search/Match: Consideration of Kβ Peaks

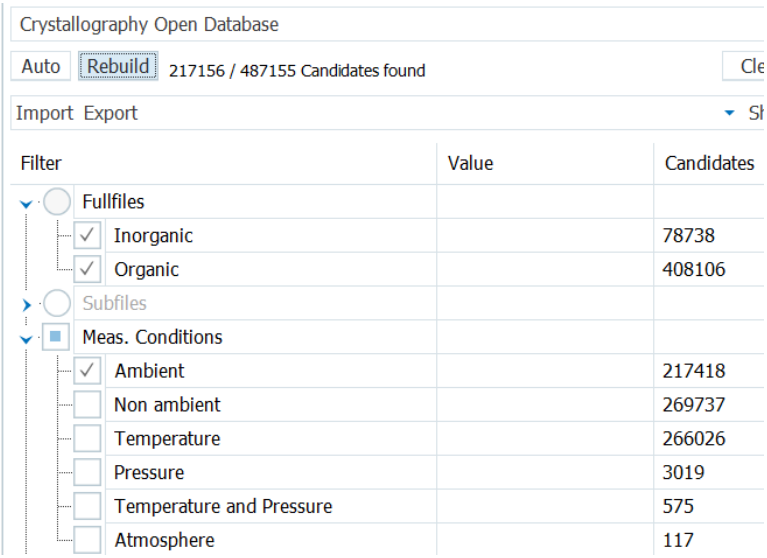
The automatic search/match algorithm takes Kβ peaks into account if the Kβ/Kα ratio is defined in the scan properties.

Search List

If an automatic search was performed and the setting "Auto-Search Results as Candidates" was selected, the likely candidates are marked green in the first column.

A new button below the search list allows exporting all search results as TOPAS structure files.

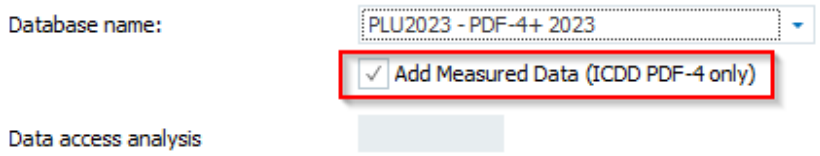
Database Filter: Measurement Conditions in PDF and COD databases



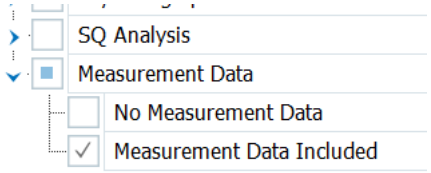
Measured Data in PDF-4 Databases

The DSRD Compiler collects all raw data which are part of the PDF-4 and places them in the precompiled files for quick access.

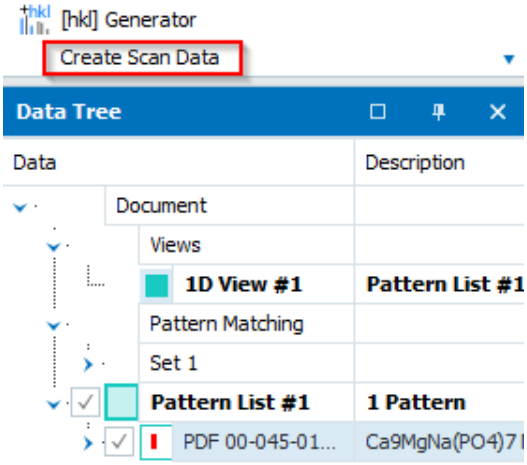
Check the marked box in the compiler to include the data:



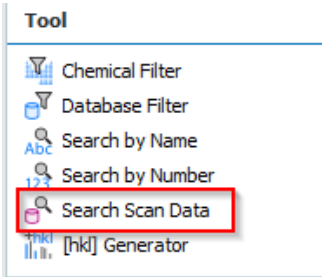
A new database filter allows extracting all patterns during a database search which have the original raw data attached:



If such a pattern is added to the document, it will have a new command "Tool | Create Scan Data" to import its raw data:



The new direct search for scans "Search Scan Data" is available on the document and scan list levels:

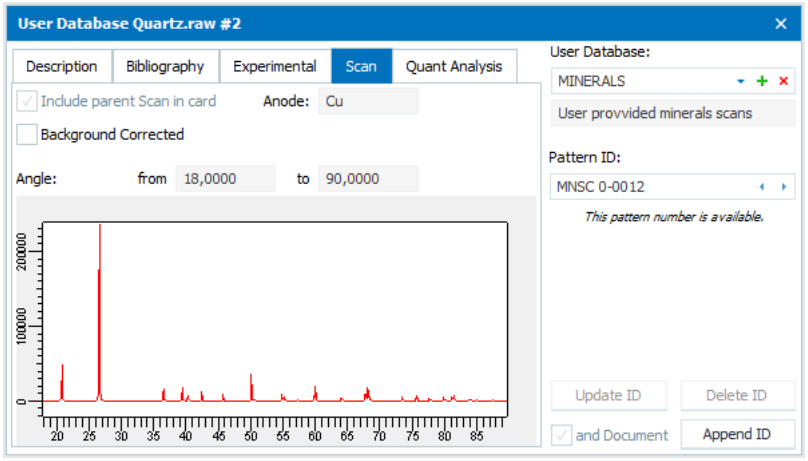


This command is also available for Pattern Matching Sets and References.

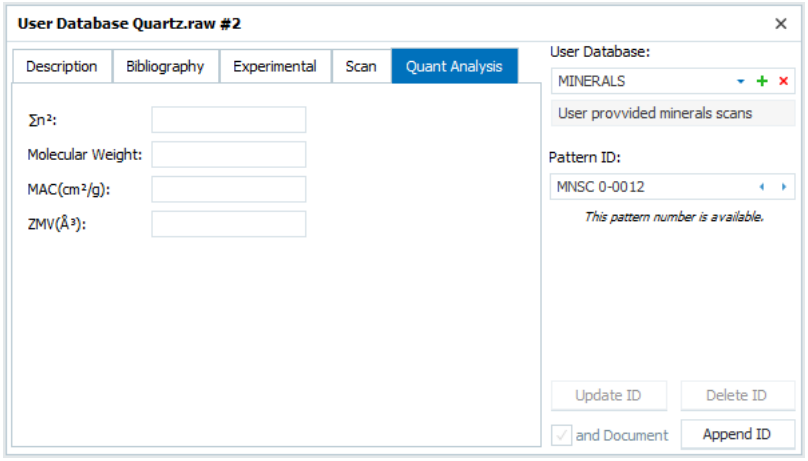
Measured Data in User Databases

The capabilities of user databases have been extended to include measured data. Consequently, user databases can be utilized to store reference measurements or other measurements of interest.

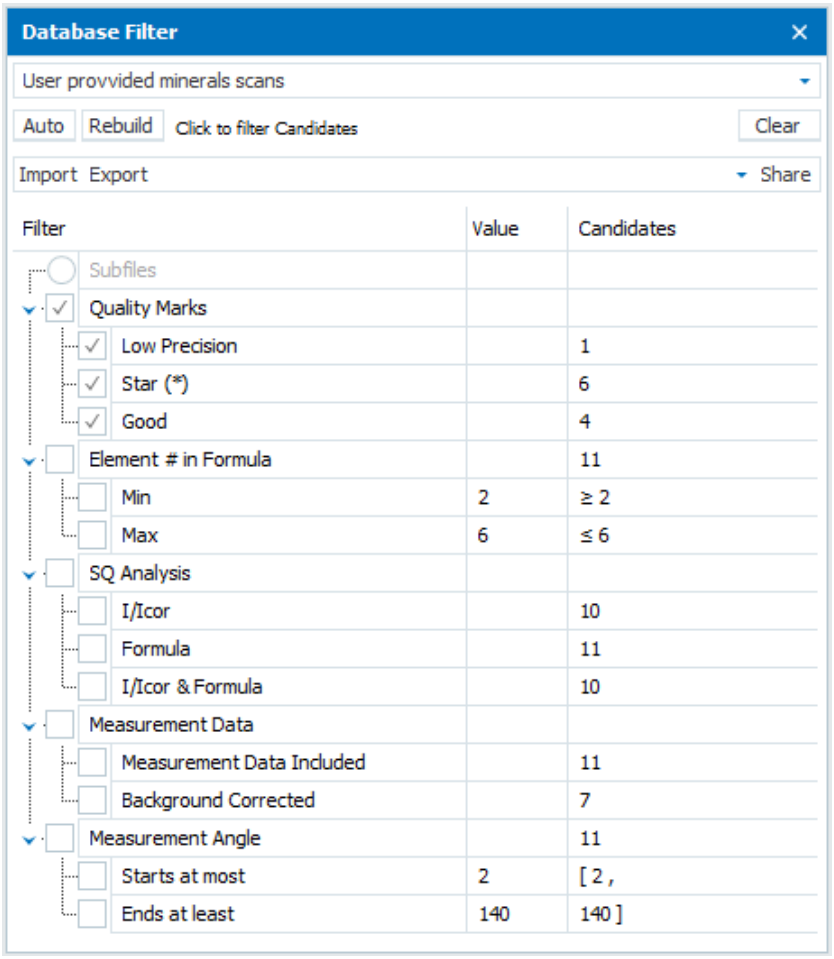
To add a scan to a user database, employ the newly available "Tool | User Database" command on the scan. The user Database tool opens with some adaptations for scans:



The scan can be marked as "Background Corrected". On the "Quant Analysis" tab some extra properties can be entered that are useful for quantitative calculations:



While searching in user databases that contain scans, filtering is possible, e.g.:

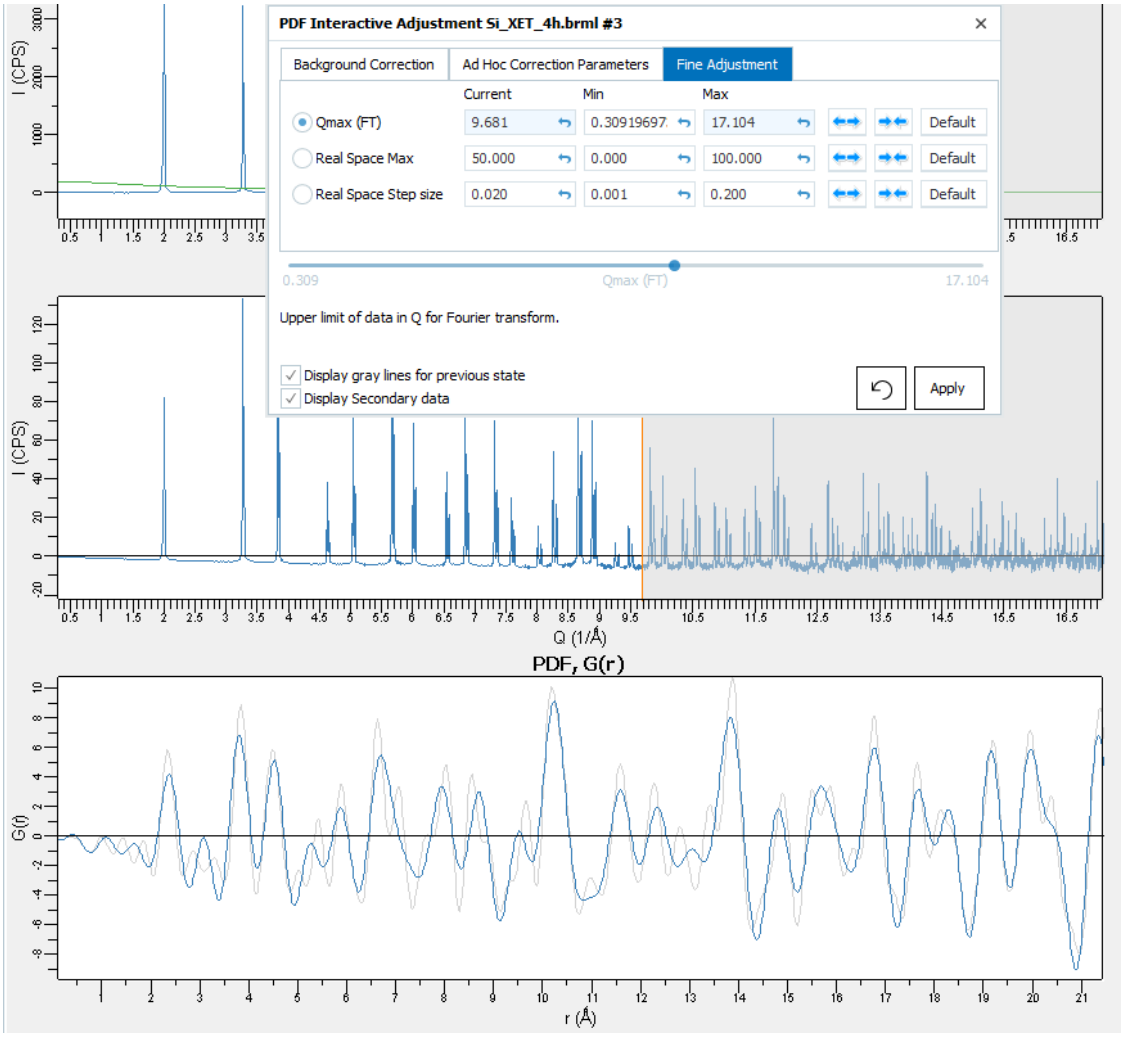


The filters are calculated dynamically depending on the provided data.

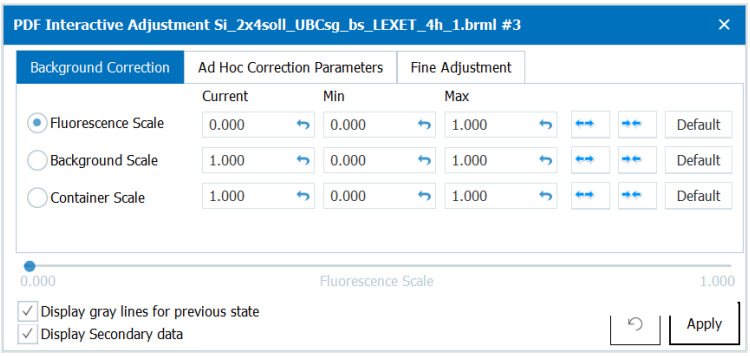
Pair Distribution Function (PDF) Processing (license level 7)

A new command "Create PDF Processing" is available for scans to calculate the pair distribution function. Measured instrument background and container data are taken into account during the calculation. The results can be exported for further calculations.

A PDF View displays three graphs including the PDF at the bottom simultaneously:



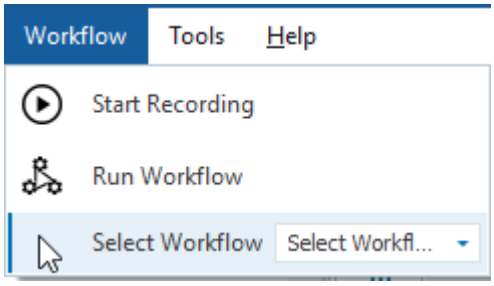
The PDF Interactive Adjustment tool allows parameter changes that trigger an immediate recalculation and display:



The Manual Addendum contains a description of the PDF processing module in EVA.

Workflow (license level 7)

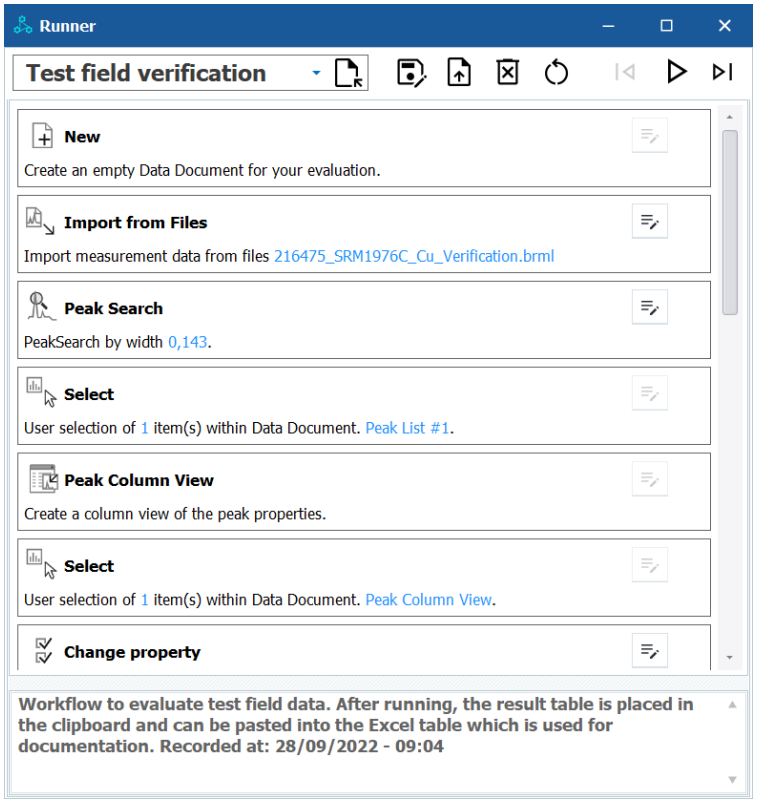
New Workflow menu commands and corresponding main toolbar buttons indicate the availability of workflows. Workflows are collections of commands which were previously recorded and can be re-played at any time.



A rich subset of more than 110 EVA commands can be recorded in workflows. While a recording is active, only recordable commands are enabled. The recording icon changes during recording. Each time a command is recorded a status message is displayed.

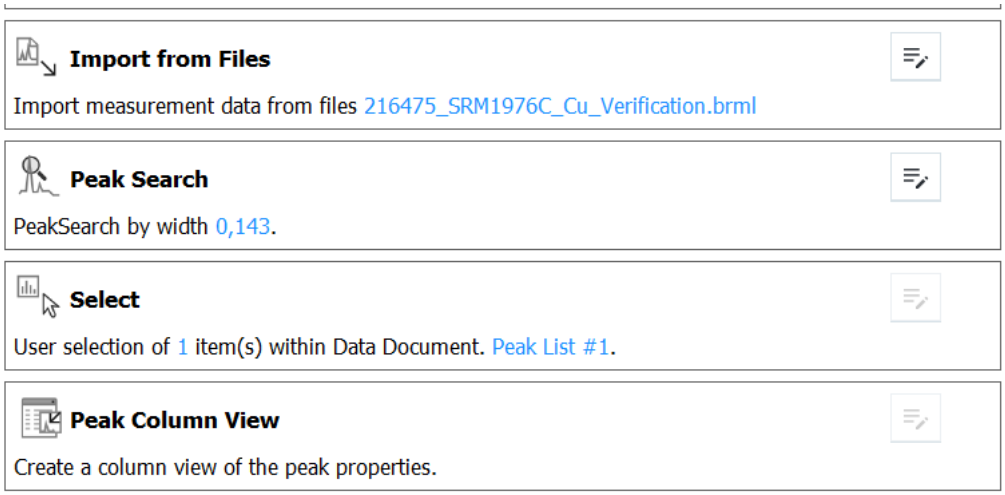
The Workflow Runner Tool

The Workflow Runner tool is the interface to control all workflow-related tasks.



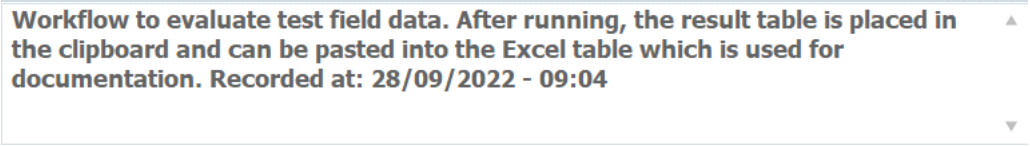
The toolbar on top of the Workflow Runner contains the workflow selector on the left side and a collection of buttons to control the workflow on the right side.

The command list below the toolbar is populated with the workflow commands after a workflow has been selected.



Command parameters may be changed in a pre-recorded workflow using the edit button on the right side of a command:

Below the command list is a guidance control that displays information about the workflow or the command under the mouse cursor:



The workflows which are shown in the runner control are context sensitive. Only workflows that start with a command applicable to the current selection in the data tree are displayed and allowed to start.

Workflow Instant Runner

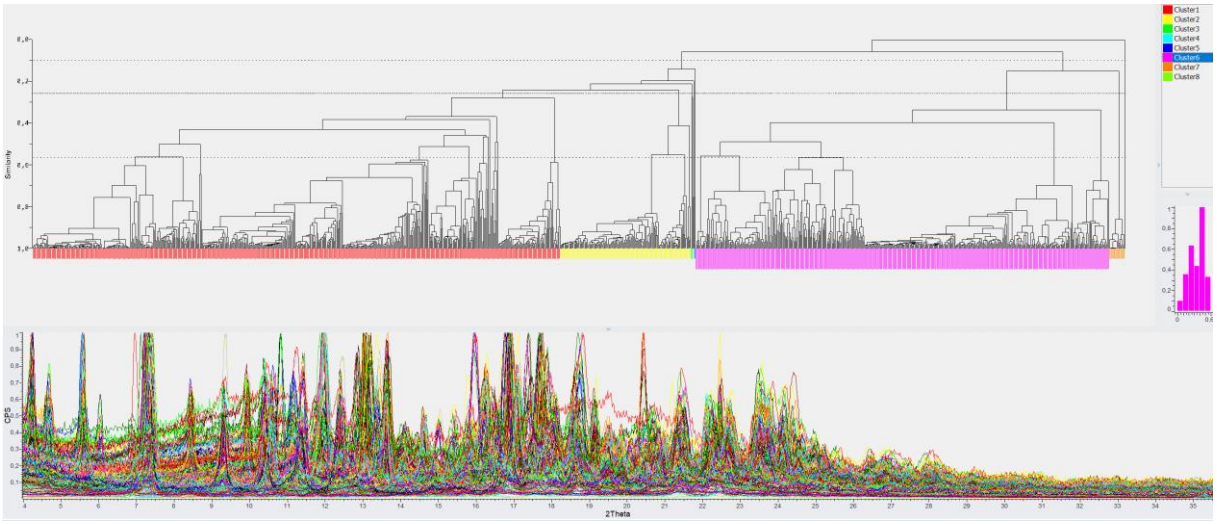
The main toolbar contains a special drop-down list that starts a workflow instantly after being selected. This list contains all available workflows. If an unsuitable workflow is selected, an error message will be displayed.

Improvements and Changes

Cluster Analysis and Dendrogram Control

The cluster analysis can be carried out for thousands of scans, depending on the number of measurement points and the available computing power.

To accommodate the larger data sets which are used in the cluster analysis, the dendrogram control has been replaced by a newly developed, much faster version.



The new dendrogram control allows for a quick display and manipulation of more than a thousand scans.

The Pattern Matching node has a new command "Export clusters script …" which generates a command line script. When this script is running, a file structure is created on the disk and the analyzed files are copied into sub-directories according to their cluster membership.

"Calculate sticks at import" Setting

If the pattern has a valid space group, the lines are recalculated. The extinction rules are observed. If the space group is missing, no recalculation is carried out.

Multiple hkls for Imported or Calculated Patterns

EVA 7.0 handles multiple hkls for pattern sticks. The hkl lists are stored and displayed (graphically and as a stick property) if the pattern was imported from the PDF or COD database and if the pattern is a result of an STR or CIF import.

To display all hkls, check "Display Alternate Indexations" in the "DB Pattern" tab in the Settings dialog.

Frames that are not Stackable by Default can be Collected in a Stacked Frame List

Holding the Ctrl key down while importing the frames will collect the frames into a stacked frame list even if all properties are similar. This will work for frames with similar axis positions and sizes.

Frame Integration for Continuously Measured EIGER Frames

The integration cursor's minimum step size for a Gamma integration is automatically set to the frame's 2Theta step size if it was originally smaller, e.g., before import or during copy & paste.

The step size for the 2Theta integration is unlimited. Use the sub-pixel integration if the integration result is jagged.

TOPAS Export

If a pattern has no unit cell, it will be exported as a peak list.

Installation Program

The installation program is an executable EXE file instead of an MSI file.

The CodeMeter software has been updated to V7.51 to include the latest security fixes.

The CodeMeter Runtime Kit installer and the Microsoft Visual C++ 2015-2022 Redistributable installer has become part of the bootstrap code to improve compatibility between different software versions. Consequently, both parts will be visible in the list of installed applications. They were not visible before EVA V7.0.

Miscellaneous

The scan has a new property: Kβ/ Kα1 ratio which is set to 0.1% by default.

The compact scan list feature has been made available for all license levels (formerly at least V6).

The Undo and Redo buttons display the affected command in the tooltip.

There is a new global setting: "Unlock intensity in the Area tool by default".

The 1D View's property "Reverse order" has become part of the default properties in the Settings Dialog, Properties tab.

Bug Fixes

- FB#4388: Wrong cursor after deleting all but one frame
- FB#19260: HKL generator does not generate all reflections for triclinic SG
- FB#21337: Wrong Measurement Duration in .raw file
- FB#21439: HKL Generator does not generate all peaks for a monoclinic cell
- FB#21789: Fixed a logic problem that caused the auto-threshold algorithm to diverge when there were many peaks barely above the noise
- FB#21793: Print preview page empty after deleting on scan
- FB#21853: Create Level tool is cut off on hires screens
- FB#21993: Problem using an exported triclinic COD structure in TOPAS
- FB#22036: Pattern sticks not on the proper scan in waterfall view
- FB#22039: After a Fourier smooth, the 2Theta end value of the smoothed scan is wrong
- FB#22072: Critical Bug in Phase ID with COD Database V6 and newer
- FB#22332: No Application for PMI Analysis Written in DB
- FB#22494: PMI Results Type for correlation
- FB#22627: Subtract Scans: do not extend the data of the difference by data of the subtrahend outside the range of the minuend
- FB#22668: Exporting/Converting multiple scans at once not working
- FB#22937: Frame View Zoom with the mouse wheel is deactivated after adding Wedge-, Slice-, Ring-, Rectangle- and Area Cursor
- FB#23053: Crash after Copy & Paste
- FB#23074: CIF export removes spaces from the Hermann-Mauguin notation
- FB#23356: DB-View not available because unit cell parameters are missing
- FB#23727: Tiny 2theta shift between the brml and the exported XY file
- FB#24016: EVA crashes when using the hkl generator on a pdf card where the compound name starts with "("
- FB#24070: Include the atomic positions when creating a user database entry from a cif or a str file
- FB#24175: Crash in Replace Scan... if more more than one scan is selected
- FB#24183: View #2 is missing
- FB#24586: *.STR Export from PDF structures - imprecise export of space group setting
- FB#24784: Synchronize the auto view for selection from different scan lists
- FB#24872: Cannot open SPECTRA*plus* XRF database
- FB#24967: Area Cursor X-Axis: 2Theta, Theta, etc. selection is lost
- FB#24973: Sticks not adjusted to the baseline of the second scan after pattern drag & drop
- FB#24968: 2D Frames: automatic frame integration after cursor import does not work
- FB#25067: Old DIFFRAC*plus* EVA documents cannot be opened
- FB#25241: 2D view of cooling segment shows wrong assignment to 1D data
- FB#25311: More tolerant decoding of composite space groups
- FB#25320: Measurement duration is too short

Version 6.1.0.5

Bug Fixes

- FB#23958: If data with a wrong Ka1/Ka2 ratio are imported, the search/match can crash
- FB#24071: Improved checks for ICDD server license
- FB#24981: 2D View is missing the "Reset Toolbar" command

Version 6.1

New Features

COD Database with Organics Sub-File and Improved Duplicates

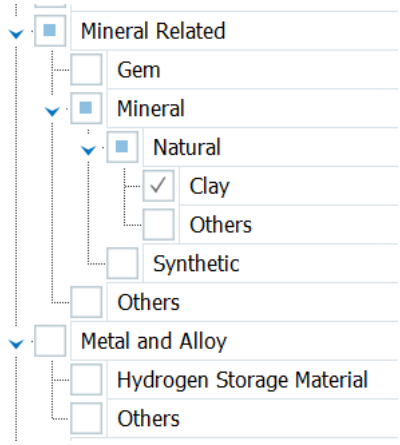
The pre-compiled COD which is available with the EVA V6.1 release has an organics sub-file and an improved detection of unusual space group notations. The duplicate phases detection has been improved.

ICDD PDF Databases with Server License and Organometallic Sub-File

EVA V6.1 can address the new server license of the PDF-4+ and PDF-4 Organics databases. This is fully automatic because the licensing is configured on the database side. EVA checks such PDF licenses regularly. A license check information is displayed in the status bar during the check.

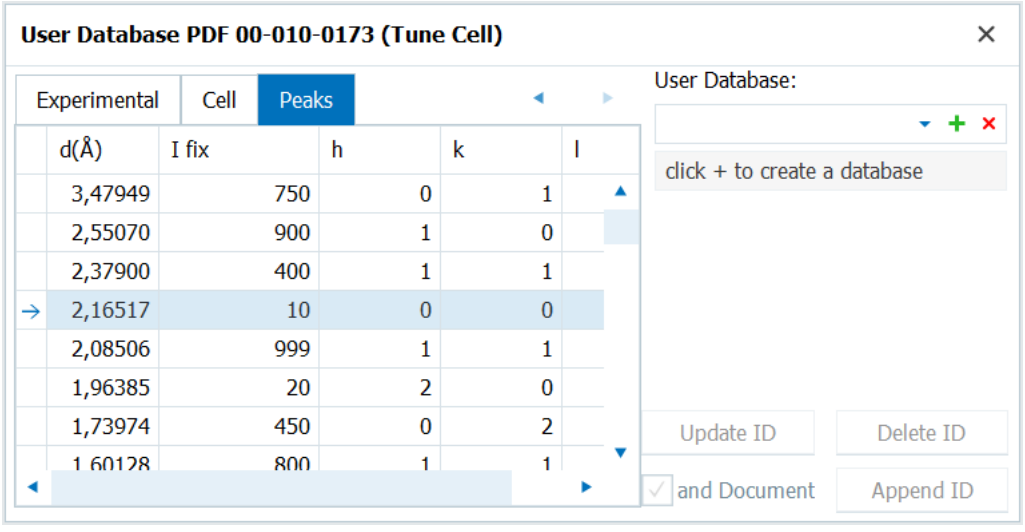
The organometallic sub-file is part of the PDF Release 2023 and is available in the database filter.

The database filter displays finely grained subsets of subfiles when they are available:



User Database Tool

The User Database tool has an improved peak list control where the details of the peaks (d, I, h, k, l) can be edited. The tool's window size can be changed to accommodate longer peak lists.



Improvements and Changes

Scan Properties

If the divergence slit opening is given in mm, it is also displayed in degrees.

Scans have a new property for the Z-KEC axis: "Z-KEC". The knife edge collimator position is displayed if it was mounted.

Scan Merge

If the merge command does not give satisfactory results, try to hold the Shift key while starting the merge. An alternative merge algorithm will be used.

X-Offset Tool

The X-offset tool allows changes smaller than 0.001° if the scan's step size is smaller than 0.002°.

Export Scan(s) with Sample ID Command

The Scan properties have a new property "Name for Export" below the "Label" which can be filled with templates that represent the scan properties. A detailed description of how to use it can be found in the manual for the Label property. If this property is filled with data, the "Export Scan(s) with Sample ID" command will use the configured name instead of the sample id.

Frame Properties

The count limits for the frame display can be set manually in the view properties. There is a new property "Auto Range" which has to be unchecked to edit the limits.

The experiment file name was added to the frame properties. It is displayed if the frame is loaded via a brml import.

Patterns

Patterns have a new property "Superspacegroup" in the case of modulated structures.

Database Filter - Crystallographic Data

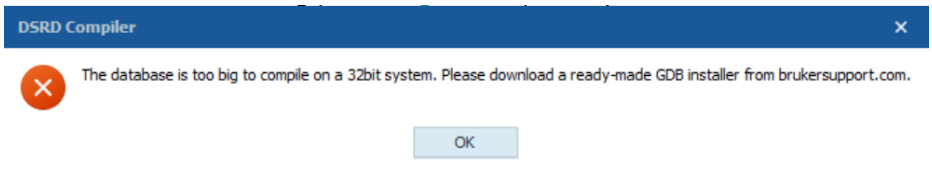
The filter has new checks for individual lattices which can be used during data mining with "Search by Name".

DSRD Compiler

During the potentially lengthy initial data analysis phase, a percentage value is displayed after the "Please wait…" message.

DSRD Compiler - Limited memory on 32bit Systems

If a recent PDF-4 database should be compiled and the free memory is not sufficient on 32bit systems, the following message will be displayed:



The compiled GDB files are available for download from the www.brukersupport.com website. Please note that you need a valid ICDD database license to use these GBD files.

Search/Match Database Compatibility

DIFFRAC.EVA V6.1 is compatible with ICDD PDF-2 and PDF-4 databases and the PDF-4+/Web at least until release 2023. It is advised to compile the databases with the V6.1 DSRD compiler to gain the new database filter functionality as described above.

Miscellaneous

When the command "Export Multi-Range Scan" is called from a scan list and a file extension other than RAW was selected, the file written was silently written as a RAW file. In that case, an information notice is displayed in V6.1.

The "Hide Shadow" property for the Waterfall view is now checked by default.

The crystallite size predicted by the Scherrer formula as part of the area properties is now given in nm instead of Å.

The CodeMeter software was updated to V7.51 to include the latest security fixes.

Bug Fixes

- FB#5349: Slice cursor missing for a single frame
- FB#6380: Set colors of integrated curves
- FB#11714: Correct status display of unfinished frames
- FB#15847: Integration takes too long for continuous frames
- FB#16910: Intensity problem for integrated cylindrical frames with cursor step sizes smaller or different than the frame's step size
- FB#19260: HKL generator does not generate all the reflections for triclinic SG
- FB#19525: Missing reflections for triclinic cell
- FB#20082: Upper Limit of Intensity Color Bar of 2D Frames may exceed 1 million counts
- FB#20727: Crash during integration cursor step size change in the Settings dialog
- FB#20925: DB View shows different values for PDF and CIF/STR
- FB#21337: Wrong Measurement Duration in .raw
- FB#21381: Center X and Center Y values in Override Detector Parameters are rounded to the nearest integer
- FB#21550: COD entries which lack the _atom_site_adp_type keyword have B=0 in EVA's search database
- FB#21761: Make Hide Shadow default for 1D View
- FB#21765: LAM File selection for .pro Export
- FB#21806: EVA crashes when performing a consecutive search by name on a pattern in an empty document
- FB#21844: Create DB view not possible for patterns with unknown unit cell
- FB#21920: Export multi-range scan in XY format creates a raw file
- FB#21993: Fixed wrong angles in STR for some symmetry-groups
- FB#22016: STR export fails when a pattern without atomic coordinates is selected
- FB#22072: Critical Bug in phase id with COD Database V6 and newer
- FB#22106: Crash in peak search for very flat scans
- FB#22116: Sub-pixels are missing for integration cursors on the stacked frame list
- FB#22164: Wrong Psi profile for EIGER frame integration, Introduce Omega offset into the Gamma-Psi conversion
- FB#22197: Microslit added to slit detection
- FB#22224: Search on single peak added, filtering works again for peak lists
- FB#22240: EIGER 2D Still/Snapshot in EVA not supported
- FB#22242: Misrouted automatic Background Correction for 2Theta-Integration of 2D-Frames
- FB#22482: Create Area tool: allow editing of left and right intensity when "Lock Int." is off
- FB#22307: EVA crashes exporting a pro file
- FB#22309: Missing data point in scan data disturbs background calculation
- FB#22307: EVA crashes exporting a pro file
- FB#22313: RAW files of suspended measurements contain zeros for the non-measured part
- FB#22316: Sub-file tree does not display more than one child level
- FB#22538: Experiment File Name missing in 2D frame properties
- FB#22549: Drives for a scan from Bragg 2D view not correct
- FB#22600: Pro file cannot be read by TOPAS if the measurement file name contains ' signs
- FB#22677: Crash in EVA V6.1 due to a very large number of data points in a scan
- FB#22713: Format of measurement duration wrong
- FB#22906: Scan export: the original file is overwritten with the exported file, if the file name was not changed
- FB#22941: Wrong Z oscillation speed from BRML
- FB#23060: Crash when the legend is changed during multi-selection
- FB#23089: VDO file not identified as coupled 2Theta-Theta
- FB#23195: Units are missing when the Slit opening is in deg
- FB#23259: Large .brml with more than 20001 data points cannot be imported
- FB#23410: Potentiostat data are not displayed correctly in 2D View
- FB#23740: When "Name document after sample id" is used, sample IDs with illegal path characters crash EVA during File Save

Version 6.0.0.8 (and 21 CFR Part 11)

ICDD PDF-2 Release 2012 and Earlier Versions

The ICDD database installation software did not install 64-bit drivers until Release 2012. Therefore, it is necessary to use EVA's 32-bit version when using PDF-2 databases until Release 2012.

Bug Fixes

- FB#21055: Fix for slow reading of a document
- FB#21861: ICDD PDF-2 Release 2009 cannot be built
- FB#21935: Crash during tab removal
- FB#21946: Crash in select tab control while searching by name
- FB#22031: Scan signature user and time mismatch in EVA printout
- FB#22471: Crash during signature reading while opening EVA file from database
- FB#22641: Peak fit results are not correctly displayed after opening an EVA file
- FB#22645: The document's evaluation time is only updated after re-opening a document

Version 6.0.0.7 (and 21 CFR Part 11)

New Features

21 CFR Part 11: New Save & Approve Command

To speed up the workflow, we have added a Save & Approve command. This allows for saving the EVA project in the database and signing it in one step. It works like the Save command with an additional request for a signing login and it requests the reason for the signature.

The save operation is logged in EVA's document log and the audit trail. The signing is logged in the audit trail as all other signing operations are.

21 CFR Part 11: New Settings for Saving EVA Files in the Database

There are three new settings to control the behavior of the EVA file saving in the database:

"Warn when an EVA file name already exists" – it prevents accidental reuse of a file name but allows it if it is intended.

"Prevent EVA file names from being reused" – EVA file names cannot be used more than once.

"Require password for EVA file save" – EVA files can only be saved in the database after entering the logged-in user's password.

21 CFR Part 11: Scans

The experiment comment, which is saved when an experiment is saved in the database by the XRD Wizard is a new scan property. It can be printed in the header/footer section of the report.

Scans that have been dismissed or invalidated are not shown in the Import from Database dialog even if the setting "Import only signed scans" is switched off.

21 CFR Part 11: Scan Clone and Replace Commands

The Scan Replace and Scan Clone commands read measurements from the database instead of the file system.

21 CFR Part 11: Import and Export Integration Cursor Commands

The Scan Replace and Scan Clone commands read measurements from the database instead of the file system.

21 CFR Part 11: Printing

There is a new parameter "User's full name who printed" which will add the user's last and first name to the header or footer of the printed document.

The "Sample comment" entered during "Start Jobs" can be printed as well.

The Settings dialog has a new check on the database tab "Print requires at least date and user". If this is checked, only print layouts will work where the user and date are configured for the header or footer.

21 CFR Part 11: Signatures

Document and scan properties: "Signature Valid" was replaced by the new property "Validation State".

The signature of the EVA data file is displayed in the properties. The signature status of any related evaluations is displayed in the Results Manager.

The scan import dialog shows only validated and approved measurements if the checkmark "Import only signed scans" is activated in the settings. Without the checkmark, unsigned measurements are shown, However, no invalidated or dismissed measurements are displayed.

21 CFR Part 11: User Rights

DIFFRAC.EVA's 21 CFR Part 11 version recognizes an extended set of user rights (all new except "Import Files") as described in the following paragraphs.

Evaluate

A user with the right to evaluate can start DIFFRAC.EVA.

If a user without the right to evaluate attempts to re-login into an open DIFFRAC.EVA the program aborts. Unsaved changes in a document are not saved.

Approve or Dismiss

EVA data files can be approved or dismissed. A user with this right can use the "Sign Database Items" and "Save & Approve" commands.

Import Files

A user with this right can import files from the file system for comparison purposes. This will invalidate the Part 11 compatibility of the document. This document can subsequently no longer be saved in the database.

Use the Undo mechanism to return to a compatible document version without the imported file.

Display Files of Other Users

A user with this right can see files of other users in the "Import from Database" and "File Open" dialogs.

Without this right, only files created by the logged-in user will be displayed.

Clear Peak Marker

Peak markers and areas can be removed.

Users without his right cannot remove peak markers and areas.

Modify Peak Marker

Peak marker properties and area properties can be changed. Peak markers and areas can be manipulated with the mouse.

Users without his right can only insert peak markers and areas but not manipulate them.

Change Software Configuration

The Settings Dialog can be used to change settings. Settings can be loaded and saved. A user without this right can only load a predefined settings file.

Change Layout

The commands Save Layout and Load Layout can be used. The window layout of DIFFRAC.EVA can be changed. A user without this right cannot change the program's window layout but can load a pre-defined layout.

Print/Export Not Approved Results

The user is allowed to print/export results which have not yet been approved.

Select Print Layout

Users with this right can select any pre-defined print layout in the document properties.

Without this right, the globally defined print layout (Settings dialog, General tab) will be used.

Modify Print Report Templates

Users with this right can select any pre-defined print layout in the print preview and can change any pre-defined print layout in the print preview. Users with this right can also select any pre-defined print layout in the document properties.

Without this right, only the print layout defined in the document properties can be used. The content of the selected layout cannot be changed.

21 CFR Part 11: Audit Trail

The column "Evaluation ID" is filled when an EVA document is saved in the database. This makes it easier to find the audit trail entries for a certain evaluation.

To avoid long single-field audit trail entries, EVA saves one entry per line. Filtering for the evaluation ID allows displaying all audit trail entries belonging to one document save operation.

Improvements and Changes

Search/Match Database Compatibility

DIFFRAC.EVA V6.0.0.7 is compatible with locally installed and licensed ICDD PDF databases and the PDF-4+/Web at least until release 2022.

User Login Window

The login window displays the application name in the caption.

Import Files from Database Dialog

The dialog has additional columns for data file id and evaluation file name. Columns for the experiment signatures were added.

Documents

The document description was converted to multi-line text. It can be used to store and print a longer text and can contain the reason for saving the document and a batch number without a limit to the text length. The text field for the description in the Save dialog was changed into a multi-line control. When a multi-line description is printed in the header/footer of the report, it is printed as a single-line text where the lines are separated by a "|" character.

Scans

Scans have a new property for the UBC collimator: "UBC Collimator Opening". The POLYCAP collimator is displayed if it was mounted.

The potentiostat attachment displays more properties: Sub Scan Number, Segment Mode, and Segment Number.

Peak Search

The Peak Search tool has a new option to limit the search to the current zoom range.

Labels

Labels can be rotated freely. A new Orientation option is available in the Label tool.

2D Integration Cursors

If the software is in database mode (mandatory operation for Part 11), integration cursors are saved to and imported from the database. Automatic integration is carried out if selected in the Settings dialog.

Bug Fixes

- FB#1862: Full Frame Cursor: Undo/Redo are not working properly
- FB#9435: If the framework logs a user automatically off, write the product name into the audit trail
- FB#10754 UBC_Collimator not listed in EVA
- FB#17072: Workaround for an issue with the Merge tool (use Shift key when Merge is started)
- FB#17361: The login window does not show the application name
- FB#17592: Make file name visible in Import from database dialog
- FB#20562: Opening a BRML file in EVA directly from Outlook is not possible
- FB#20607: CTRL Z issue with some tools
- FB#20832: New wait form to fix the issue with the "Initializing EVA" form not disappearing
- FB#20981: Missing threshold refresh in Background tool
- FB#20993: Undo after peak Search closes the EVA document
- FB#21118: Font Header / Font Row (Properties -> Printing) does not respond to property changes
- FB#21164: Open Scan in EVA Button (in Results Manager) should not import invalidated or dismissed measurements
- FB#21170: Y-axis rescaling for zoom reset
- FB#21190: Printed legend too small on hires screens
- FB#21196: Info messages about peak fit do not disappear after the project close
- FB#21199: Special position incorrect for TOPAS export
- FB#21217: Error during compilation of file-based PDF databases
- FB#21273: Importing in-progress measurements should display only the measured points
- FB#21375: Fill in the scan's user comment during printing
- FB#21411: AXIOM and PDF-4/WEB databases should use the new duplicates algorithm
- FB#21412: DSRD compiler cannot compile older databases
- FB#21426: Wrong merge
- FB#21451: Merge error "index out of bounds"
- FB#21498: Difference Audit Trail should be written
- FB#21528: Add timing info for sub-scans with seconds in the display
- FB#21531: Crash after Replace Scan
- FB#21534: Crash during EVA document save on a network drive
- FB#21545: Create Area French and German localization dependent tool size
- FB#21585: Crash after leaving the filter cell in a column view
- FB#21588: EIGER 1D data that are not completely measured are not displayed properly
- FB#21589: DB filter on document node missing database selection
- FB#21595: No automatic integration after cursor import from the database
- FB#21601: Crash in Normalize command
- FB#21672: UBC collimator with Montel optics is not displayed in frame properties
- FB#21933: Create a DIF from the HKL generator when no scan is active causes a crash
- FB#21993: Problem using an exported COD structure in TOPAS, "null" Wyckoff symbol removed

Version 6.0

New Features

New Automatic Search/Match Algorithm (all license levels)

The automatic search/match algorithm has been rewritten to provide good results for real-life applications. Many internal improvements have been applied which makes the automatic search applicable for routine use. The algorithm is very fast on modern multi-core computers because it uses parallelized, multithreaded code.

There is an option in the settings on the Database tab "Auto search as candidates" which allows using the new automatic algorithm the same way as the manual algorithm, i.e., the candidates are not already selected after the search.

Automatic Search/Match on cement samples

Cement samples are difficult to analyze because of the multiple strong peak overlaps. The best results can be achieved if the database filter is set to "Cement" and "Mineral related" as well as all qualities except "Hypothetical" and all statuses. Using the chemical filter for cement may help but may also suppress minor phases which can occur infrequently.

The Search/Match FOM (Figure of Merit)

During the search, potential candidates are selected from the reference database following user-set parameters and the declared filters. These parameters and filters are set in EVA's Search/Match toolbox. A Figure of Merit (FOM) is calculated for all potential candidates having at least one line falling in a region of non-zero intensity.

The FOM of a pattern is a computed figure that reflects the equivalence of the pattern to the measured diagram in comparison to the set of measured peaks by using the internal search criterion. It is qualitative matching information, that is neither directly related to the likelihood of the actual presence of this phase nor to the possible percentage of it in the mixture.

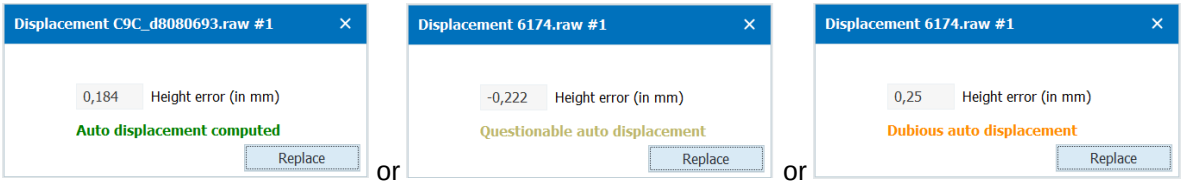
The FOMs are the same in manual and automatic search algorithms, however for manual operation the search results are sorted by decreasing FOMs, whereas the automatic search can select other phases or other variations of the same phase that have a lower FOM but a better match of peak positions/intensity. Therefore, after an automatic search, the results are generally not sorted by decreasing FOMs, nevertheless, the major phases usually have higher FOMs than the minor ones and appear before the latter.

FOMs do not only depend on the patterns but also the scan. It is therefore not possible to compare FOMs for the same pattern found on different scans.

The traditional DIFFRACplus FOM, where the lowest value was the best value, has been replaced by the new value. The new value is 100% for a dummy stick pattern that perfectly explains the unknown scan. As a result, the new FOMs are more informative than the traditional FOMs.

Automatic Displacement Correction after Search/Match (license level 6)

While performing an automatic search/match, an attempt is made to calculate a displacement correction automatically. If a potential displacement is detected, information is displayed with the calculated displacement and a quality description:



By clicking Replace, the displacement is applied to the scan and used for further analysis.

If "Dubious auto displacement" is displayed in the dialog, it should only be accepted if the analytical results appear to be correct.

The feature can be switched on in the scan properties under Corrections: "Enable Auto Disp.". This is also part of the global scan properties in the Settings dialog.

Please note that as soon as the displacement dialog is displayed, the scan property "Enable auto displacement" is reset, even if the displacement was not accepted. For using the auto displacement function for further searches, it must be checked again in the scan's properties.

The "Enable auto displacement" property has no function for scans with an angular range less than 50° and is therefore not displayed.

Search/Match Databases and DSRD Compiler

The DSRD compiler has been extended internally to calculate a better duplicates table. Compared to former versions, more duplicates are found which improves the search/match. The DSRD compiler is multithreaded as well to speed up the time-consuming duplicates calculation.

The PDF-4+ Web which fetches the database entries from the web has been updated to accommodate the 64-bit DIFFRAC.EVA version. An updated PDF-4 Web 2021 installer with 64-bit compatibility is provided by the ICDD to become compatible with DIFFRAC.EVA.

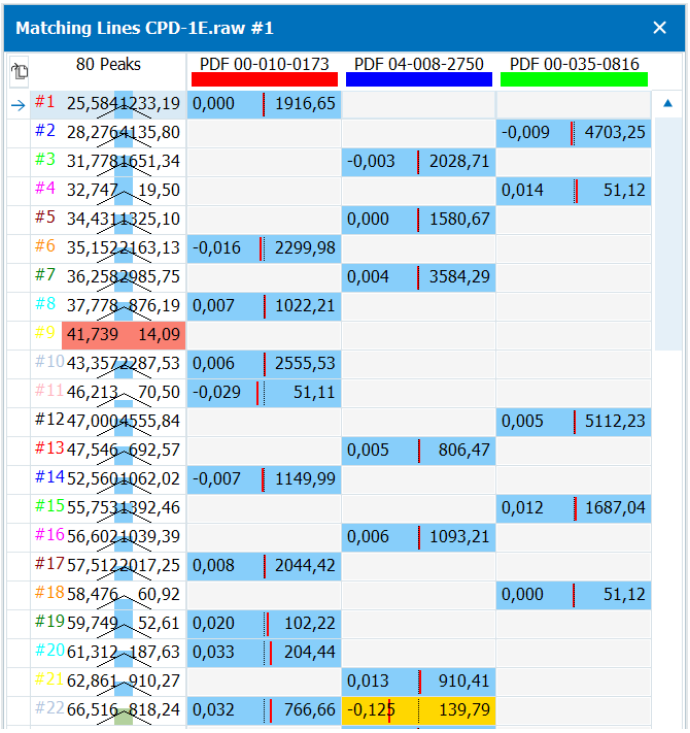
It is now possible to compile the Crystallography Open Database (COD) directly from the web. Bruker provides an initial database on the installation medium and as a download, which can be extended at any time by the customer. The time to update the COD depends strongly on the age of the installed COD. It can vary from about 30 minutes to several hours.

EVA V6.0 installs a reduced COD database containing only mineral phases (>13000) in the DSRD6 folder. A fully compiled COD is available from the installation medium or as a download from Brukersupport.

Every installed database requires a hard disk space between 5GB for PDF-2, 12 GB for PDF-4+, 22 GB for PDF-4 Organics, 2 GB for PDF-4+ Web, 5 GB for a COD search database only, and 24 GB for a full COD including the crystal structure files (all Release 2021). Using an SSD (solid state disk compared to a classic rotating hard disk) as a system disk is advised for a very fast database search.

Matching Lines Tool (license level 6)

For users who are interested in how well individual peaks are matched by the search results, an automatic Matching Lines Tool was added to EVA. The tool window is created by the "Matching Lines" command on a scan node. If a scan has a peak list, this view is automatically filled with peaks. As soon as patterns are added to the scan, each pattern creates a column in this view. To use this tool, a peak list must be created manually, e.g., with the peak search tool.

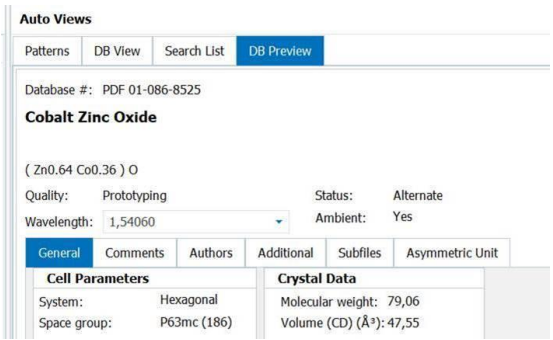


The entries for the pattern lines contain the difference between the line position and the peak position, and the line height. The background color indicates the match quality for the peak. A color that changes from blue to green to yellow means that a match is good, average, or bad. A red color means that there is no matching peak in the peak list. In addition, a black vertical line in the middle of the cell indicates the peak position and a red line indicates the line position. The distance between the two lines reflects the quality of the match position, as does the background color. If only the red line is visible, it indicates that the angle position is a perfect match. If the line position and the line height match, the background should be blue.

The left column in the view contains the peaks with a number for the position and the counts. If the peak has a match, its background should be transparent. In the middle of the entry, there is a colored bar which is the average color of all the lines that match that peak. It indicates the angle-matching quality. The tip of the small roof-like graph indicates the actual peak height. The height of the bar represents the sum of all the line counts for that peak. The difference between the height of the bar and the tip of the roof reflects the quality of the counts match. A bar that just touches the tip is a perfect counts match. If the peak is not matched by any pattern, its background color changes to red.

New DB Preview Tab in Auto Views

An additional DB Preview tab is shown when the search list is displayed. This tab shows the search list's selection, while the DB View tab shows the selection in the data tree:

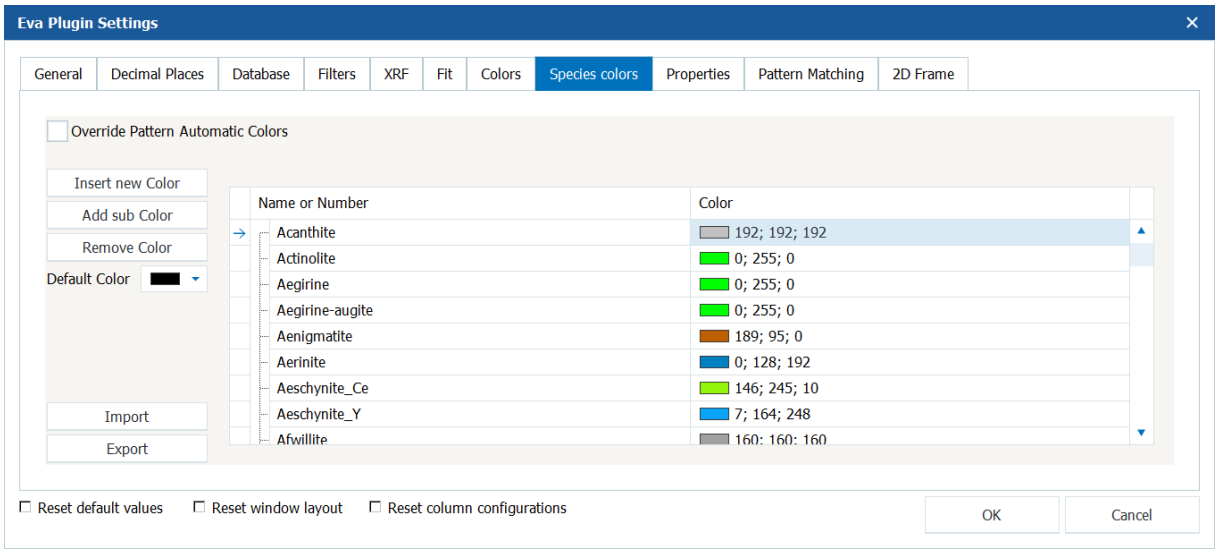


A double click on the DB Preview tab adds the current selection to the data tree and creates a persistent DB View in the EVA document.

Phase (Pattern) Colors according to Bruker AMICS and other Schemes

Bruker AMICS is an automated mineralogy system for SEM and comes with pre-defined phase colors.

A new page "Species Colors" in the Settings dialog allows choosing from predefined color sets or creating an individual color scheme:



The color scheme can be exported and imported. Pre-defined sets are available in the tutorial folder for Bruker AMICS and FEI mineral colors.

TOPAS Project File Creation from a Scan Node (license level 6)

A TOPAS project file (*.pro) can be created from a scan node. The scan data and the patterns with either a unit cell or a crystallographic structure are converted into a TOPAS project file for a quick quantitative analysis or unit cell refinement. If a pattern does not contain at least a unit cell it is ignored during export and a warning is displayed.

There are two optional scan properties related to the TOPAS file creation, the "Emission Profile" and the "Instrument Parameters". Both entries can contain a file path to an emission profile file (*.lam) or an instrument parameter file (*.par) which are used instead of the data given in the scan properties.

Remark: EVA files created with older versions than V6 do not contain structural information and need to be re-created with V6 for TOPAS export.

Evaluation Results are stored in the DIFFRAC.SUITE Database (license level 6)

EVA stores the following evaluation data in DIFFRAC.SUITE database tables when an EVA project is saved:

Scans:

- Crystallite size
- Fitted sum and difference curves if a fit was performed

Areas
- Net area
- Position maximum
- Position center of gravity
- Left angle
- Right angle
- Left intensity
- Right intensity
- FWHM
- Integral breadth
- Chord middle
- Raw area
- Net intensity
- Gross intensity
- Crystallite size
- S/N ratio
- S/N ration sigma
- P/B ratio

Peaks
- Position
- Net intensity
- Gross intensity
- Miller indices hkl

If a fit was performed:
- Peak function
- Area
- Crystallite size
- FWHM (low/high for asymmetric peaks)
- Shape (low/high for asymmetric peaks)
- Fitted peak curve

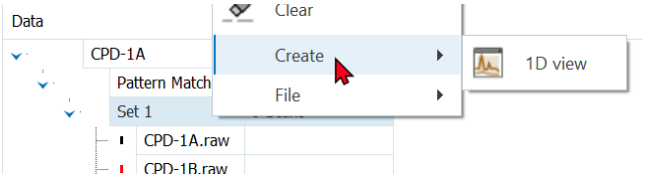
Patterns
- Pattern name/database number
- Quality
- I/Icor
- Crystal system
- Space group
- Lattice parameters
- Density
- Volume
- Color
- SS/FOM
- Stick positions and heights
- Fitted pattern curve if a fit was performed

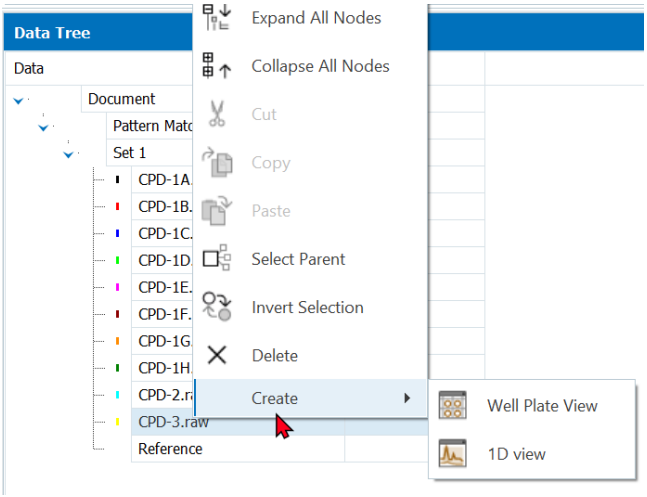
Open EVA from Results Manager

If buttons for measurements and evaluations have been configured in Results Manager, EVA can be opened with the selected database entries directly from the Results Manager. For details, please consult the Result Manager manual.

Pattern Matching

There are new commands available to create 1D Views and corresponding scan lists from the pattern-matching Set node and individual file nodes:





SnapQuant

This external tool allows a quick SQUALL or PMI calculation with a small GUI or it is used online after the measurement. It requires an EVA file that contains a set of reference samples on which a SQUALL or PMI has been performed previously with EVA. Any unknown which is part of the EVA file is ignored during the SnapQuant run.

For online evaluation, select the EVA file and the SnapQuant or SnapQuantPMI script. The results of the online evaluation are stored in the DIFFRAC.SUITE database and can be visualized with the Results Manager.

Lab Notes View

A text property has been added to the document which can be edited with the new Lab Notes View, to be created from the document node. The purpose of this property is to store information collected while working on the document which does not fit into the short document's description property.

Skin

A new flat skin "Bruker 2020" was introduced.

Improvements and Changes

Scans

Scans have a new Line Thickness property. This was introduced mainly for presentation purposes because all lines with a thickness greater than one are much slower drawn than the hardware-accelerated lines with a thickness of one. For lines with a thickness greater than one, we do not support other line styles than a continuous line.

Additional scan properties are recognized for:

- New TRIO slit mount
- New EIGER 2 R 250k detector
- New Spinner rotation stage
- New non-ambient properties for a potentiostat attachment

2D Frames

The integration step size for the integration cursor can be saved as a default property.
If frames are loaded by their accompanying BRML file, the UBC collimator is displayed in the frame properties.

Manual Search/Match

The manual search/match algorithm benefits from improvements made for the automatic search like better duplicate detection, which may result in slightly different search results compared to former EVA versions. The search speed was improved using parallel processing (CPD-1D, no filter, 2nd run: V5.2: 5.3s, V6.0: 0.7s; CPD-1D, minerals filter, 2nd run: V5.2: 2.2s; V6.0: 0.4s; PC: DELL XPS 15 9570).

Search by Name

The Search by Name tool now also accepts numbers as part of the search string, like "Muscovite 2M1". To use this functionality, the search databases must be compiled with V6 EVA's DSRD compiler.

Search/Match Database Filter

To accommodate the search for patterns with crystallographic structures, the filter had an entry "Crystallographic Structure" in V5.2 to select only patterns having atomic coordinates. For clarification, this filter has been renamed to "Atomic Coordinates and Unit Cell".

The other entry in the group was called "Unit Cell" until V5.2. Selecting this filter retrieved all patterns with a unit cell, regardless of if they had atomic coordinates or not.

To make searching easier, this entry has been reworked and renamed to "Unit Cell without Atomic Coordinates". The filter will only allow patterns with unit cells but without atomic coordinates. Selecting both entries in V6 will retrieve all patterns with unit cell and atomic coordinates as a union.

Like other parts of EVA V6, the database filtering has been sped up by parallel code execution.

Search/Match Database Compatibility

Due to changes in the internal database structure, it is required to recompile the PDF databases with the DSRD compiler which is part of the V6.0 installation. Please note that older EVA versions are not able to access these newly compiled databases. Therefore, the default storage for the compiled databases has been changed to "C:\ProgramData\Bruker AXS\DSRD6". This folder can be changed during a custom installation.

DIFFRAC.EVA V6.0 is compatible with the ICDD PDF databases at least until Release 2021.

Area Tool

A signal-to-noise calculation was added. The value for sigma can be entered.

Large Measurement Set Import Speed

The loading speed for measurements is nearly 4-fold compared to V5.2 which will speed up applications with large non-ambient data sets. The time to display was sped-up by about 50%.

Loading EVA files with many data nodes was sped up as well. The improvement depends on the kind of objects in the tree and reaches a factor of 10 for certain node configurations.

XRF Results Import

SPECTRA.ELEMENTS database compatibility

There is a new selection on the XRF tab in the Settings dialog which allows selecting a SPECTRA.ELEMENTS database. If such a database is chosen, subsequent XRF imports are taken from this database.

SPECTRA^{plus} database compatibility

EVA's 32-bit version can import data from V1 and V3 *.mdb databases, and the recent *.accdb databases. The 64-bit EVA V6 version can import only from *.accdb databases. The prerequisite is a Microsoft Access database engine from 2010 or later. This database engine must be installed as a 32-bit version for 32-bit EVA and as a 64-bit version for 64-bit EVA.

Miscellaneous

It is now possible to switch between open tools with the keyboard commands "Ctrl+Left" or "Ctrl+Right". Tools can be closed with the "Ctrl+F4" key combination.

Bug Fixes

- FB#1882: 1D view creation from list of scans performance improved
- FB#2048: Import individual scans from multi-scan files into different scan lists if necessary
- FB#3331: 2D view reset (zoom, color level) changing a 2D view property
- FB#3417: Turk Regional parameters destroy the DSRD filtering system
- FB#3869: Slow mask change for 2D frames
- FB#6391: Last selected view should be focused automatically (special case after peak insertion)
- FB#9873: 2D frame integration step size change not recognized
- FB#11288: Sorting does not work correctly for Scans in the Auto Views table
- FB#11637: EVA 5 merging files problem (XRR/HR measurements)
- FB#12163: Save cell info and structure from DIF to User DB
- FB#12430: No data on ROI for EIGER measurements is shown in EVA
- FB#13133: User database - no feedback when using "Append ID"
- FB#13377: Side view in 2D view: negative sign barely visible
- FB#14576: Axis offset disappeared for Omega-2Theta BRML file
- FB#14813: Area tool switched back to V3 behavior
- FB#15777: Aberrant tool doesn't find spikes in integrated 2D frame data
- FB#16006: Show sub-scan number as scan property
- FB#16726: FOM color coding fixed for small values
- FB#17000: Multimethod-mapping: too many scans
- FB#17042: Recognize Locked-Coupled... scans as 2Theta in xy(e) files
- FB#17465: EVA freezes if it momentarily loses the license
- FB#18178: After clicking "Override Detector Parameters" the 2D frame selection is lost
- FB#18269: No 2T_nc drive in EVA for LE0D scans
- FB#18440: Cannot open 1-step measurement in EVA
- FB#18820: After Fixed Step-size rebin wrong step-size is displayed for the original scan
- FB#18832: Recognize data on motorized TWIN optics
- FB#18992: Information on Goebel mirror as part of TWIN is lost in EVA
- FB#19022: S/M results are different when searching a DIF several times (without/with Auto)

- FB#19058: Replace and Clone scan forced in database mode
- FB#19064: Area tool speed improved
- FB#19269: No 2T_nc drive in EVA for LE0D scans
- FB#19324: No phi position for LE 0D 2T_nc scan
- FB#19339: Error saving results to the database
- FB#19421: File damaged message instead of a file locked message when loading BRML
- FB#19425: Sample rotation for FLIP-STICK in RAW file is wrong
- FB#19502: Missing x, y coordinates imported from *.xy-Files created by Auto-2D-Integration
- FB#19508: Crystallinity calculation and amorphous display not working
- FB#19509: Crash while importing (large) multi-range file
- FB#19510: Fix for CIF angle export; allow STR and CIF export for patterns without atomic coordinates
- FB#19537: "Background subtracted" property not checked for background corrected data display
- FB#19560: Area Tool unresponsive on multi-range data
- FB#19597: Non-Ambient parameters not transferred to sub-scans of repeat-PSD
- FB#19671: SQ results do not change after pattern fit
- FB#19775: Wrong duration time for 2D continuous EIGER measurement
- FB#19776: Time per step per pixel added for frame files if available from the BRML
- FB#19878: Non-ambient parameters not changing for multiple EIGER scans from the same segment
- FB#19940: Incorrect background calculation for variable slits below 5°
- FB#19912: Prevent Overflow exception in 2D control
- FB#20045: Temperature units (°C) are lost
- FB#20083: Synchronous sample rotation display fixed for RAW files
- FB#20093: Wrong name of scintillation detector for RAW files
- FB#20119: Loading an alpha_i scan takes too long
- FB#20203: EVA displays negative measurement duration
- FB#20292: Problem with crystallinity calculation
- FB#20427: Deleting a large number of scans or other objects takes a long time
- FB#20448: Moving a level manually on 1D View is very slow
- FB#20483: The Cement filter doesn't have the non-cement elements excluded
- FB#20513: Data leftovers removed from the status bar
- FB#20557: The Aberrant tool isn't working properly
- FB#20562: Opening a BRML file directly from Outlook is not possible
- FB#20583: Search pattern by number gets wrong intensity if "Calculate missing sticks at import" is active
- FB#20665: Error after changing default properties for 2D Frame
- FB#21000: Search by name not searching properly (special characters/wildcards)
- FB#21094: Crash when "Save to PDF" in Print Preview tries to write over an already existing write-protected file

Version 5.2.2

Bug Fixes

- FB#20339: Crash during EvaPlugin.Activate due to a float overflow in a user database
- FB#20371: Crash during Addition/Subtraction if Display Amorphous was set in the default properties

Version 5.2.1

Bug Fixes

- FB#19991: Area calculation wrong after opening an EVA file if scans with variable slits and a manual change of the area are carried out
- FB#20081: Problem with area display on scans with variable slit after a manual change of limits
- FB#20339: Crash during EvaPlugin.Activate due to a float overflow in a user database
- FB#20371: Crash during Addition/Subtraction if Display Amorphous was set in the default properties

Version 5.2

Improvements and Changes

Scans

Scans that were most likely converted from another format and older RAW formats allow setting the slit mode manually to account for measurements with variable slits.

Scans exported in xy(e) format have four digits for the angular position and three digits for intensity values.

The scan list's name can be configured in the default properties.

The scan's "Job ID" was called up to V5.1 "Database ID". To avoid misunderstanding it was renamed to "Job ID" in the scan's properties and to "JOBID" as a macro for the labeling.

Patterns

Newly created Kβ patterns have the same color as the original (Kα) pattern but with less saturation. There is a new command to create a $WL\alpha_1$ pattern which also results in a pattern with the same, but less saturated color.

1D Views

If the Shift key is pressed during scan import, scans that become part of the same scan list do not open a 1D View containing all scans of the list, but open individual 1D Views for every scan in the list.

2D Frames

If the Shift key is pressed during the 2D frame import, frames that would normally be sorted into a stacked list and displayed as a stacked view will be placed in individual single frame lists and a single 2D Frame View will be opened for each frame.

In case only one frame is contained in a list, no thumbnail view is created anymore.

When the frame display is zoomed in until the individual counts are displayed, the counts have now one decimal digit to accommodate frame corrections made after the measurement.

Frames are stacked if the difference in x, y, or z is below 0.01mm (was 0.05mm in V5.1).

Search List

Until V5.1 the number of matching and non-matching lines included the Kα1 and Kα2 lines. Starting with V5.2, we only count the Kα1 lines.

Search/Match Databases

Due to changes in the internal database structure, it is advised to recompile the PDF databases with the DSRD compiler which is part of the V5.2 installation. Please note that older EVA versions may not be able to access these newly compiled databases.

DIFFRAC.EVA V5.2 is compatible with the ICDD PDF databases, release 2020.

A search for phases containing Greek letters is working if the Greek letter is spelled like "ALPHA" for the α character.

Tool Windows

If the tool height allows, the slider adjusts to the height for easier movement.

Default Properties

The scan list's name which is displayed in the data tree can be configured in the default properties in the Settings dialog, Properties tab. The default is the scan-axis name.

The stick's captions have been added to the default properties.

Miscellaneous

A text property has been added to the document which can be edited with the new Text View, to be created from the document node. The purpose of this property is to store information collected while working on the document which does not fit into the document's description property.

21 CFR Part 11 Related Changes

The document's signing status is displayed in the document's properties.

The "Peak" object in the menus and the audit trail has been renamed to "Peak Marker" to avoid confusion with measured peak data.

Status line messages are no longer displayed if EVA runs in Part 11 mode. To get the messages displayed in Part 11 mode, use "Display additional error details" in the Settings dialog, General tab.

Starting with the measurement software V7.5.2, the user's right to "import files" which is part of the lab manager's set of rights controls the ability to import and export files from and to the file system.

Two columns for sample ID and job ID were added to the audit trail. They are filled when measurement results are imported. More parameters are recorded in the audit trail.

While in former versions every action in EVA created one audit trail entry, V5.2 saves only one audit trail entry when an EVA file is saved to the database. This will make the audit trail inspection easier.

EVA V5.2 does not sign evaluations in the database automatically when an EVA file is signed with the "Sign Database Entries" dialog. Evaluations must be signed in the Results Manager. The signing of EVA files (not individual evaluations like peak fit results) has to be done in EVA's "Sign Database Entries" dialog. It is no longer possible to sign EVA files in Results Manager.

Importing files from the file system for comparison purposes is restricted to users who have the privilege "Import Files".

The document property "Last Write User" was renamed to "Last User" and the print macro "DOC_LASTWRITEUSER" was renamed to "DOC_LASTUSER" accordingly. The "Evaluation User" is set to the currently logged-in user when the document is created or opened. The "Last User" is set to the user who was logged in when the document was written. The evaluation and last user differ if the EVA file was saved by a different user than the currently logged-in user.

Bug Fixes

- FB#1882: 1D view creation from list of scans performance improved
- FB#5316: Set the scan's step size after a fixed step size re-bin
- FB#7065: Incorrect log scaling for 2D frame limit control
- FB#7501: Make the position and size of the database import/open dialog columns persistent
- FB#13130: Area tool - clear fields to avoid confusion after "Append"
- FB#13792: Missing peaks from STR import
- FB#14197: Peak Fit: improve view after zoom - the hyperbolic background was not taken into account

- FB#15057: 2D display for unfinished measurements has too many y positions
- FB#15563: Add tilt stage drives Zeta and Xi
- FB#15578: Trim the integrated data to avoid y-scale jumps in the cursor preview
- FB#15727: Replace scan in DB mode calls file menu but not DB
- FB#16030: Missing or additional peaks in the pattern when using "calculate missing sticks at import"
- FB#16222: If a scan didn't share at least one 2-theta point with a child pattern, the view became illegal after a zoom reset (wrong axes), 2nd fix
- FB#16341: Wrong intensity after applying hkl generator
- FB#16376: Background was not cloned after replacing scan, the sum and difference curves were wrong
- FB#16379: Crash when choosing wavelength checkbox in automatic view for a pattern
- FB#16403: Missing peaks from CIF import
- FB#16413: Normalization in 1D View fixed
- FB#16445: 'Datafile ID' property should be invisible in case of using an older measurement database
- FB#16516: Calculated crystallite size does not change if the instr. width is changed
- FB#16601: Crash when decoding chemical formula
- FB#16603: Fix a calculation bug that caused Ka2 peaks to be interpreted as Ka1
- FB#16604: Crash during peak search
- FB#16614: Pattern has blank intensities when imported into an EVA document
- FB#16629: Search entries made in the Search List's Find feature should appear in the history drop-down list
- FB#16645: Search on an empty document - wrong info displayed in database filter
- FB#16667: Adding phases after a search/match on a peak list crashes EVA
- FB#16711: Cannot do search/match on xy VCT data
- FB#16736: Wrong unit cell angles with STR Export; leading equal sign on lattice parameters removed
- FB#16767: Crash when navigating matched results (formula issue)
- FB#16771: 1D View "copy as bitmap" command does not work properly - the bitmap is cropped or too small
- FB#16910: Intensity problem for integrated cylindrical frames with cursor step sizes smaller than the frame's step size
- FB#16929: Peak Search Tool/ Default button can malfunction on slow computers
- FB#16956: Error in area calculation for very small peaks on the shoulder of a large peak
- FB#16999: Improve file grouping after import
- FB#17006: Full frame cursor for cylindrical frames does not process sub-pixel information
- FB#17017: STR & CIF import calculate angles wrong for non-Cu wavelengths
- FB#17042: Scan axis for created XY files after automatic integration should be 2Theta
- FB#17095: Document name and last used directory not set during EVA file loading
- FB#17113: Incorrect stick intensity of imported structures
- FB#17225: Index overflow in Search by Name if a Greek letter is used
- FB#17296: User Database: The author entry is not saved in "author", a search for an author is not possible
- FB#17323: Crash using scan tools when label list moved above scan in the data tree
- FB#17325: 2D view corrupted after a change of Y axis from Index to Phi
- FB#17340: Save should work like Save as and ask for a comment to allow storing customized information like batch number
- FB#17350: Add tool parameters to audit trail where missing (background, peak positions); duplicate entries for scans and patterns removed
- FB#17353: Print "document creation user" is always empty
- FB#17355: Make "Save As" invisible in Part 11 mode
- FB#17356: Remove multiplets from peak search
- FB#17357: Mention the "result filename" in the help tooltip for the "File Name" property
- FB#17359: EVA installation guide needs an addition for Part 11 where it is mentioned that "Custom" needs to be clicked
- FB#17363: Lock instrument radius in Part 11 mode
- FB#17403: Add the hkl values for the sticks in the user database
- FB#17439: Problem with COD installation when another DSRD path is used than the default path
- FB#17472: Language change: issue with auto restart when changes are not saved

- FB#17509: Wrong weight values for Match options should be rejected
- FB#17511: Crash while scrolling through the search list
- FB#17518: Crash when selecting consecutive area limits on top of each other
- FB#17545: EIGER frame is flipped
- FB#17604: Audit trail information for peaks created from peak search is incomplete
- FB#17622: Error values in exported XYE files are not correct for variable time data
- FB#17716: Variable slit correction applied twice after import for RAW files in V3 format
- FB#17763: EIGER 2D NOUT integrated data should not show Counts
- FB#17848: Asymmetric unit display wrong for the pattern if several patterns are contained in a list and at least one pattern has no atomic coordinates
- FB#17880: Crash at inserting the first pattern in an empty document
- FB#17880: STR files with c-style comments were not recognized
- FB#17946: Scan in extended view is missing when a logarithmic axis is selected
- FB#17958: Audit trail: Missing data tree object name after certain actions
- FB#18033: Wrong goniometer radius in properties for D2 measurements
- FB#18056: Sorting of columns containing numbers not done numerically in Scan View
- FB#18184: Problem when creating new pattern matching views: the new view is not selected
- FB#18210: For high DPI screens or screen scaling > 100% the size of the graphic in print preview is too small
- FB#18234: Strange looking 2D View when background is subtracted
- FB#18247: Manually added peaks are always added to the first peak list regardless of selection
- FB#18267: Missing action info in data tree and audit trail in Part 11 mode
- FB#18276: Error message when exporting a file with "Z_HTK1200" axis
- FB#18288: File/Database import from a scan selection below the Pattern Matching node is not correct
- FB#18333: Certain actions in Eva make Eva files in 'Sign Database Entries' disappear
- FB#18345: Problem with the 'Sign Database Entries' dialog
- FB#18351: Signing status is not correctly displayed in properties
- FB#18361: Signing issue if an EVA document imports multiple jobs

VERSION 5.1

User Manual and Tutorial

The additions and changes that occurred after print are described in the "DIFFRAC.EVA Manual Addendum" which can be accessed from the start menu or DIFFRAC.EVA's help menu.

New Features

ICDD WebPDF-4 Database (all license levels)

Starting with V5.1, EVA can compile and use the WebPDF-4 database. After compilation, the database access is as fast as with a locally installed search database. Internet access is required to check for a valid license.

Crystal Structure Export (license level 5)

Patterns that have a crystal structure attached in the PDF-4 databases are read with their structural information into the EVA document starting with V5.1. These patterns have two new commands: "Export Cif..." for the export in the CIF format and "Export Str..." for the export in the TOPAS STR format.

Tools Menu (all license levels)

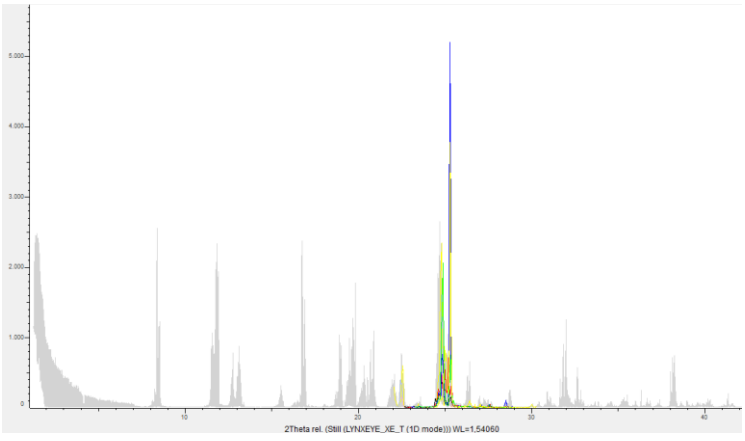
The Tools menu has two new commands: "Save/Load Toolbar Layout". They allow saving/loading the 1D view's toolbar layout. Give a short description as file name during saving and EVA will add its own additions to recognize the layout later.
The Search by Name command was made available for patterns and pattern lists.

HRXRD Measurements (all license levels)

Starting with V5.1, EVA can display HRXRD measurements measured either with linear detectors or 2D area detectors.

Compact Scan List (license level 5)

If measured data are read which contain a large number of scans, the traditional scan list is not the fastest way to work with. EVA V5.1 therefore introduces a "Compact Scan List" which reads the data much quicker and creates only one scan list node and a corresponding 2D View very fast, even for thousands of scans. If one opens a 1D View from a compact scan list node in the tree, the outline of all scans is drawn in grey and the in the Auto View selected scans are drawn as colored lines:

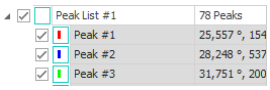


From inside the 2D View, it is possible to open the scans of interest into a second scan list with an attached 1D View by using the context menu (see below, paragraph "2D View").
For performance reasons, the side view is not available if a compact scan list is displayed in the 2D View.

Data Tree (all license levels)

The data tree has a new "Invert Selection" command which applies to the selection below a node.

In addition, lists have a new check box that can be used to select or deselect all child nodes:



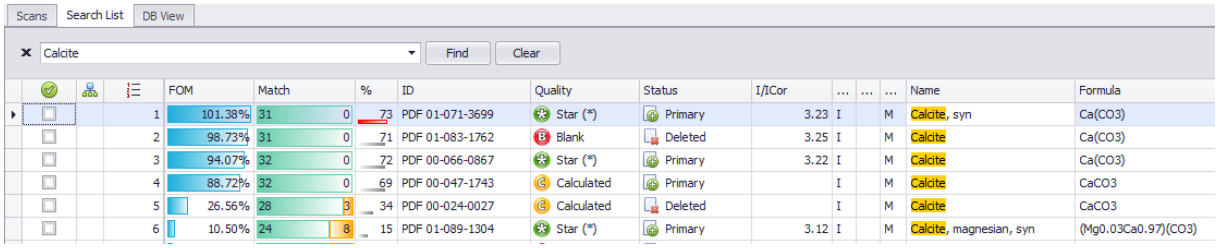
Double-click anywhere on the list entry or on a child node has the same effect as a click on the check box.

There are two new commands available – "Expand All Nodes" and "Collapse All Nodes" – which should improve the data tree handling for large documents.

New Find Feature in the Search List

When the Search List is active, pressing Ctrl+F on the keyboard opens an additional filter tool:

After entering the search term, the list is automatically filtered:

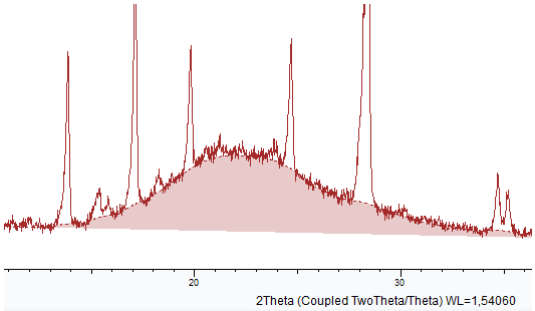


Filter texts can be not only pattern names, but also quality, status, formula, or any other text which may be worth filtering.

To ease the filter access, an additional button has been placed below the list:

Amorphous Content from a Scan's Crystallinity Calculation (all license levels)

If the crystallinity calculation is selected and the new property "Display Amorphous" is checked, a shaded background area is drawn to visualize the amorphous content:

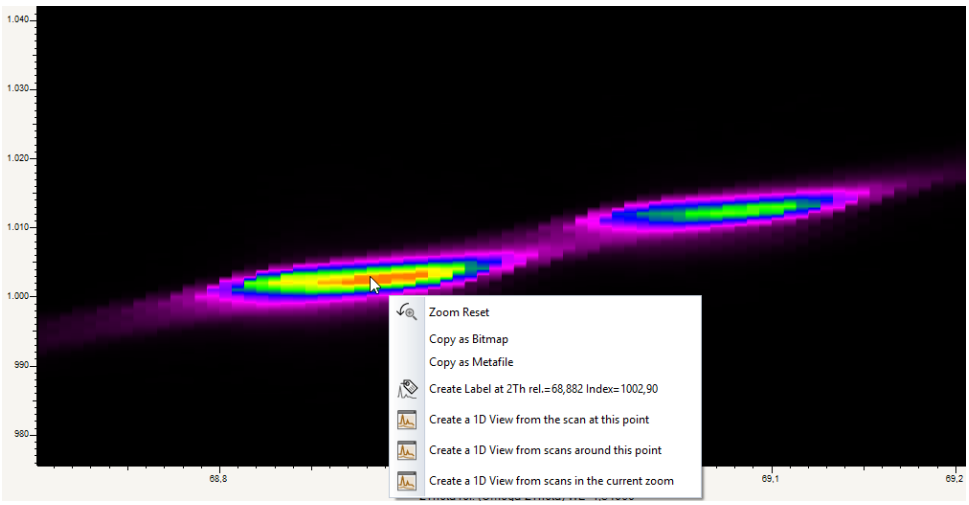


Amorphous Content in S-Q Analysis (all license levels)

The semiquantitative analysis adds a pattern named "Amorphous" automatically to the pattern list if one pattern is marked as added reference. The pattern's S-Q value is the calculated amorphous content. A shaded background area is drawn to indicate the amorphous content. The drawn area is symbolic and not dependent on the actual S-Q value.

2D View (all license levels)

The 2D View has a new feature to display the selected scans. If scans are selected in the data tree or the automatic list, the 2D View shows colored rectangles on the right side for the selected scan and a ghost line parallel to the x-axis.
Selecting scans is possible from the 2D View by double-clicking. Selecting multiple scans is possible by using Ctrl and double-clicking to extend the selection.
The 2D View's context menu has three new "Create a 1D View from ..." commands to inspect the scans of interest:



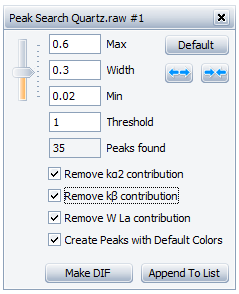
Improvements and Changes

Scans

"Scans" can be measured with only one point per scan. EVA does not open empty 1D Views for such measurements anymore but a Scan View which displays the data point in text form.
The goniometer radius was made a default property to be easily set for scans that do not have a goniometer radius stored.
If the setting "Name the document after the first loaded measurement's sample ID or file name" is selected, a replaced scan sets the document name with its sample id or file name, if the sample id is not available.
The background tool speed was improved over V4.3 and V5.0. This will be especially noticeable if the background is modified for several scans in parallel.

Peak Search Tool

The peak search tool was extended to detect $K\beta_1$ and W $L\alpha_{1,2}$ peaks:



[hkl] Generator

The [hkl] Generator tool has a new Replace button which is active if the tool was started from a pattern. Clicking Replace closes the tool.

Peak Fit Auto View

A column was added on the Peak tab to display the peak's integral breadth. Another column for the intensity in CPS is shown if the 1D View is switched to CPS.

Peak Fit Calculated Curve

A fitted peak's calculated curve can be exported into a xy file using the new "Export Fitted Peak(s)" command. If the command is applied to a multiple selection or peak list, the sum curve is exported. The same command is also available for a pattern, where the whole set of peaks is exported as a curve.

Peak Fit Tool

The peak fit tool was redesigned so that the buttons are visible on all tab pages.

If parameter limits are reached, a warning is displayed in an alert window and the session log.

2D Views

The rendering algorithm´s performance was improved. Potentially jagged edges in case of varying start values per scan were removed.
To open a 2D view, the scans must contain at least 10 measurement points.

Dendrogram View

A property "Show shade" was added to control the cluster shading.

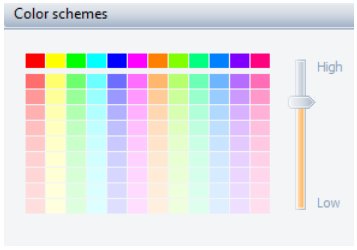
2D Frame

The code for conversion into psi scans was modified to handle psi values around 0° and psi < 90° and > 90° correctly.
Frames with extensions "._br", "._ff", and "._fl" can be read, too.

Pattern Matching Node and Views

The Pattern Matching node stores now the parameters for the minimum and maximum of detectable phases locally in the EVA file. Therefore, **older EVA files must be updated for V5.1 if they contain a used Pattern Matching node**.

The pattern-matching views have a new color selection tool implemented in the Settings dialog:



Pattern Matching Quant Algorithm

The algorithm was improved to yield better quantitative results.

Drag and Drop in the Data Tree

While it has been possible to drag single data items to a new place in the tree until V5.0, it is now possible that multiple objects of the same type can be dragged and dropped in another position of the data tree.

ICDD PDF Databases

The release 2019 contains new formulas for which the decoding algorithm was improved. Therefore, any previously compiled database should be re-compiled with the DSRD compiler.

Note: PDF databases which were compiled with the V5.1 DSRD Compiler are not compatible with previous EVA versions!

COD Database

The COD database was updated to the January 2019 version.

Bug Fixes

- FB#2693: Y-offset does not work for background corrected scans
- FB#4266: Search/match chemical filtering bug because of weird character in the formula
- FB#4518: Improvement of the layout of 3D views in Report Writer View
- FB#5232: Y-offset is not as expected in the case of simulated slits
- FB#7056: Incorrect log scaling in EVA's 2D view
- FB#7691: Strange display of str file together with raw/brml scans
- FB#8283: Extend the [hkl] generator to transport all unmodified properties to the resulting pattern, if started from a pattern
- FB#8723: Logarithmic projection in 2D view is not working properly
- FB#9838: Frames with extension "._br", "._ff", and "._fl" can be read
- FB#11890: Missing file extension when saving an evaluation file in Results Manager
- FB#12689: Print Preview: Apply button causes shrinking of Quant View
- FB#13002: Material-related info (DIF pattern) cannot be entered anymore
- FB#13101: Merge of 221 scans fails with too large end angle
- FB#13130: Crystallite size not calculated consistently in the Area tool
- FB#13189: Legend in "Copy Bitmap"/ "Copy Metafile" different size to display
- FB#13230: Saving to raw converts "Coupled" to "TwoTheta"
- FB#13256: Print preview called from a view's tab should only preview the actual view
- FB#13469: Wedge Cursor integration problem
- FB#13855: Error in the embedded format string of Chinese translation
- FB#14277: Pattern Chart view shows only 1 of 2 phases
- FB#14423: In case a "scan" with only one point is loaded, a Scan View is opened instead of a 1D View
- FB#14732: Match List not accessible if a pattern is selected
- FB#14735: Frame View gets empty despite frame presence
- FB#14756: Match List should be accessible from Pattern node/Patterns as well
- FB#14767: SQ analysis: update problem in Auto Views after a change of y-scale
- FB#14771: Settings: Maximum number of results does not work correctly
- FB#14772: Error message when saving an Eva document to a V5/V6.5 Alaska DB
- FB#14778: Update view legend after replace scan command
- FB#14782: Search/match – Chemical Filter: Explanation for colors improved
- FB#14794: Wrong CPS for exported scan obtained from measured repetitions
- FB#14804: Peak positions of a hidden scan are set to 0°2θ upon reading from the .eva file
- FB#14806: Crash in the search result list when the program is closed with the "x"
- FB#14812: Files measured with IuS tubes do not display the correct tube current
- FB#14818: Copy / Paste of a scan within a document does not apply displacement correctly
- FB#14822: 2D view of discontinued (in 2theta) scans
- FB#14856: 'Add' does not correctly add scans
- FB#14858: 'Accumulate' does not correctly accumulate scans
- FB#14941: BRAGG 2D view: Delta Omega wrong by a factor of 2
- FB#15011: BRAGG 2D View: Index out of bound error
- FB#15063: Wrong reflections with hkl generator
- FB#15109: Modified Gamma to Psi Conversion after 2Theta-Integration of 2D-frames
- FB#15154: "Cannot open XRF database" error fixed
- FB#15275: Axis offset missing in Eva
- FB#15335: EIGER 1D still: can't open brml in EVA
- FB#15378: New illegal chemistry formulas in PDF Release 2019
- FB#15404: Problem with the 'Create Level' tool
- FB#15425: Peak fit wrong for data with high background
- FB#15441: Crash during creation of a 2D View from a sequence of 0D still scans
- FB#15442: Error at the import of raw files with older file format
- FB#15517: Switching to Chinese crashes the program
- FB#15569: Forbid updating Cursor Preview for mask cursors only
- FB#15570: Can't integrate rectangle curser - grey the Integrate button
- FB#15595: Resolution loss in accumulated BRAGG2D; index overflow fixed
- FB#15607: Crash in DSRD Compiler with PDF-2 Release 2009
- FB#15637: Make all W wavelengths available for patterns in EVA
- FB#15664: Incompatibility of "Animated fit" with the pattern fit

- FB#15752: Default DB/Chem. Filter does not show up in the S/M window although defined in the Settings
- FB#15773: Display the correct info in the status bar when 2D View is active
- FB#15861: Area tool not closing properly after creating an area for multiple scans
- FB#15931: Make newly created sticks fittable
- FB#16030: Problem with missing/additional peaks in the pattern when using "calculate missing sticks at import"
- FB#16091: Crash exporting ThetaF scans into RAW
- FB#16161: VSS data cannot be fitted properly
- FB#16198: Peaks missing in a fit, if fit zoomed is used
- FB#16199: Merge algorithm to merge integrated scans from 2D frames takes a long time
- FB#16222: If a scan didn't share at least one 2-theta point with a child pattern, the view became illegal after a zoom reset (wrong axes)
- FB#16255: Peak fit: sum curve for multi-sample peak fit elevated
- FB#16233: Multiple stackable frames are sorted into two separate lists instead of one
- FB#16248: Fix for lower peak width limit for very narrow peaks; parameter values made editable for pattern fit
- FB#16252: Pattern fit: x shift limits are not obeyed
- FB#16288: Append Area: Instr. Width and K cannot be modified in the tool
- FB#16327: The sequence of columns in the Search List is not memorized
- FB#16374: Graphics update of pattern curve for a manual model change
- FB#16410: "Use alternate patterns" is no longer available in the settings
- FB#16413: Y-scale factor after normalization should be 1 for the scan with the highest intensity
- FB#16433: Peak behavior should be consistent during insertion
- FB#16435: Tune Cell, hkl Generator, "d x by" should trigger calculated pattern redraw
- FB#16476: Pattern fit does not work if the compound name is used for the pattern list's Data column

VERSION 5.0

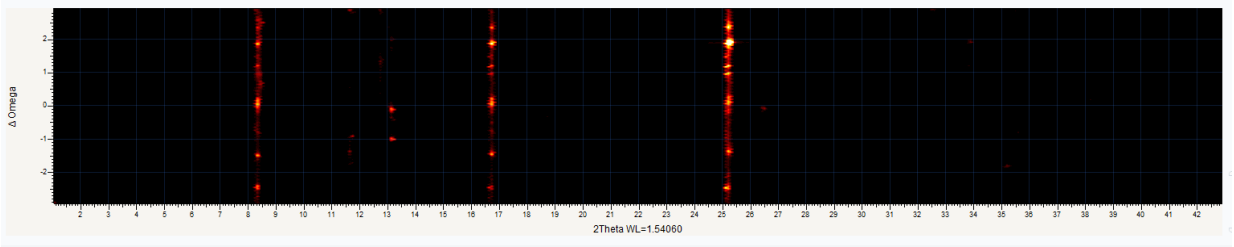
User Manual and Tutorial

The additions and changes that occurred after print are described in the "DIFFRAC.EVA Manual Addendum" which can be accessed from the start menu or DIFFRAC.EVA's help menu.

New Features

Bragg 2D View (all license levels)

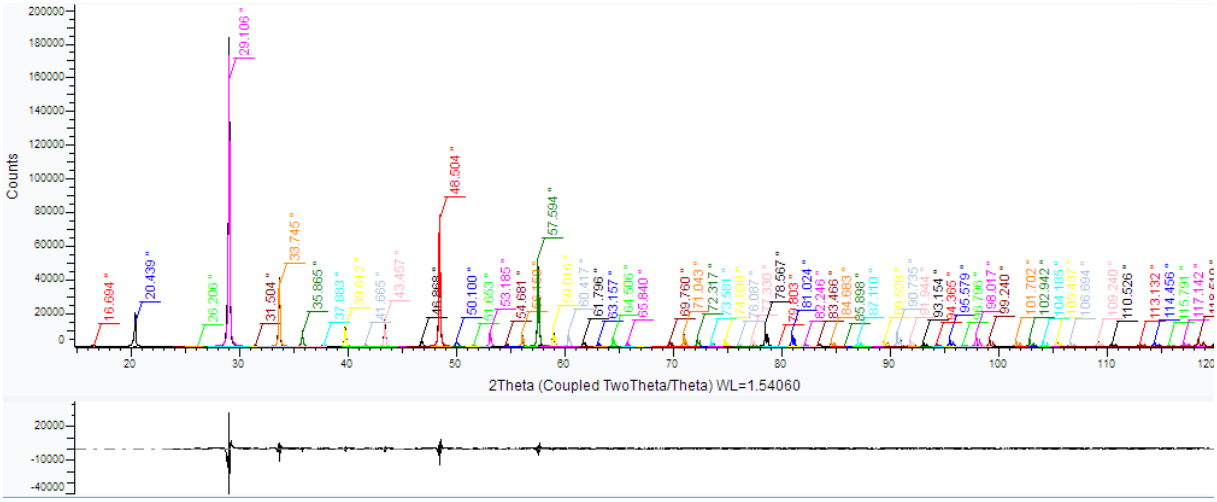
EVA displays the recently invented Bragg 2D View after executing the command "Bragg 2D Realign" on a suitable scan list:



Peak Fit (license level 5)

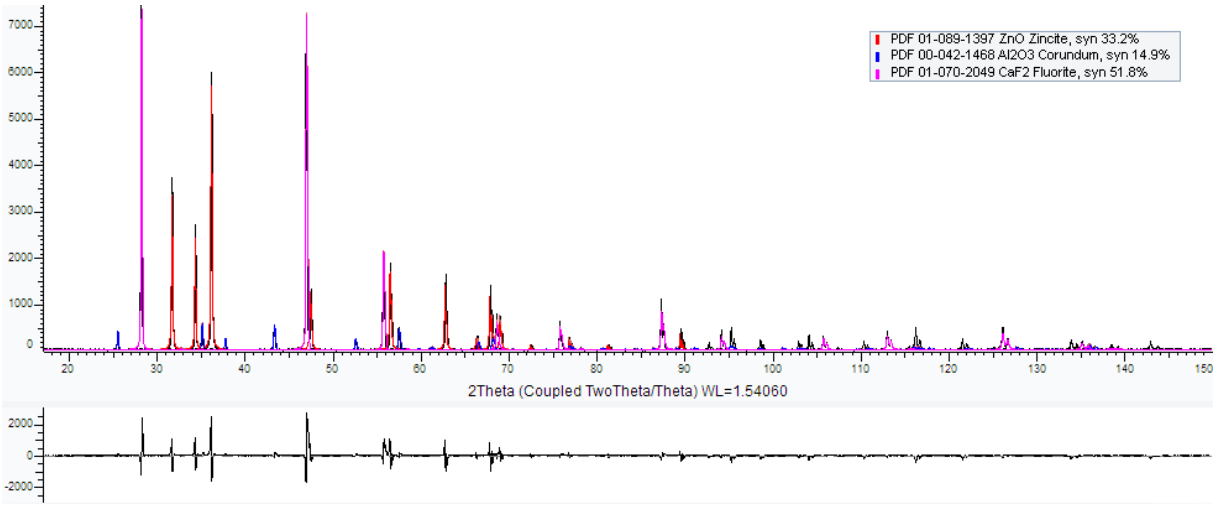
Starting with DIFFRAV.EVA V5.0, peaks can be fitted. There is a new fit tool available for a scan that allows controlling the fit process and displays the fit progress graphically. There is also a new toolbar button for the peak fit available.
The peaks have the following new properties in case of fit is allowed:

- Peak Type (Lorentzian, Gaussian, Pseudo-Voigt, split Pseudo-Voigt)
- Position
- Area
- Intensity (net)
- FWHM
- Integral Breadth
- Width (low)
- Width (high) (only for asymmetric Pseudo-Voigt peaks)
- Shape (left) (only for Pseudo-Voigt peaks)
- Shape (high) (only for asymmetric Pseudo-Voigt peaks)



Pattern Fit (license level V5)

Starting with DIFFRAC.EVA V5.0, a pattern can be fitted to be used in the semi-quantitative analysis. Fit parameters are the pattern's Scale and X Shift.



Search/Match (license level V5)

During Search/Match work, it often happens that an unexplained peak does not attract any reasonable phase. It is possible to define this peak as a preferred peak for the search/match or in short words as a **Match Peak**.

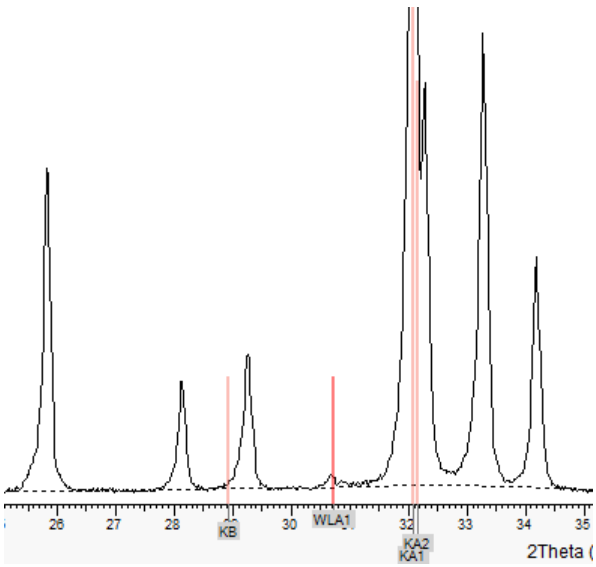
Search Databases (all license levels)

All locally installed ICDD databases (PDF-2, PDF-4 variants) are supported until the Release 2019. The new ICDD **PDF-4 AXIOM** search database is fully supported by DIFFRAC.EVA V5.0.

1D View (all license levels)

The lambda cursor which was introduced in V4.3 for search/match is now generally available for the 1D View with a tool button: 

Holding the shift key while the lambda cursor is active will display a legend for the individual lines:



Database Storage (license level V5)

In addition to saving EVA files into the database provided by the measurement software, evaluation results like SQ results are also stored in the database's compound table. The Results Manager (part of the measurement software) can be used to display these results.
The following data lists have a new "Save to database" check in the properties: Scan Lists, Pattern Lists, Peak Lists, Area Lists, and Element Lists.

The following data are saved to the database:

- Scan: Crystallinity
- Pattern: SQ result
- Peak: Position, Area (if available from fit) or net Intensity, FWHM (if available from fit), Crystallite Size (if available from fit)
- Area: Area, FWHM, Crystallite Size
- Element: SQ result

The quantitative results from the pattern matching can be stored in the database as well.

The properties' database storage can be controlled in detail with customizable flags and database compound names.

Import of XRF Data from Instruments which operate SPECTRA.ELEMENTS (e.g. S2 PUMA)

To use the "Import XRF Results" command with instruments like S2 PUMA, the compound list of the sample in question has to be exported using the Results Manager's export functionality. The results must be exported in CSV format.
In the EVA Settings dialog, XRF tab, the "User selected file" option is required. In the "Open an XRF results filename" dialog, "CSV files" should be selected to see the exported files.

Improvements and Changes

Scans

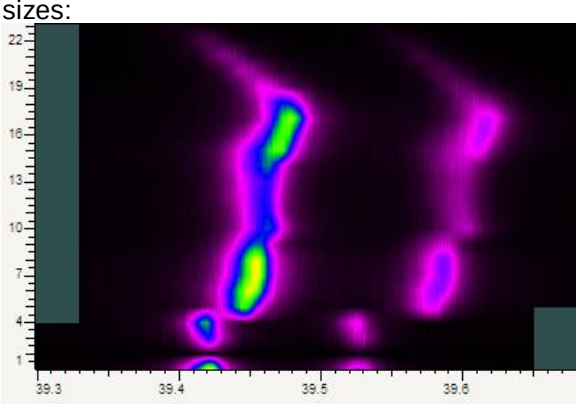
The method name {NAME} was replaced by {SAMPLEID} in the default scan description.

1D View

A log scale lower limit was added to the Settings dialog, Tab Decimal Places.

2D View

A 2D View created from a scan list can now display scans with different angular ranges and step sizes:



The selector for the 2D View's y-axis displays only the variable scan properties.

Search/Match

A full search by name on an empty document is now possible. The "remove duplicates" check was removed for the Search by Name command. The grouping led sometimes to the impression that important patterns were missing.
The Search by Name command on the document node allows filtering.

Database Filter

The database filter was reorganized to reflect the selection state better when the user switches between full files and sub-files.

Peak Search Tool

A check box was added to allow applying default colors. The Kα2 removal check is automatically set for scans with a 2Theta axis and a Kα1/2 wavelength pair in the scan properties.

User Database

Cell parameters from imported structures are now stored in the user database.

Patterns

The pattern properties display the ICSD, CSD, NIST, or LPF numbers if available.

Printing

The dotted and dashed line styles can be printed. In older versions, they were printed as solid lines.

Column Configuration

There are pre-defined configurations according to the property groups for scans, patterns, peaks, and areas. If a configuration is selected, it replaces the former configuration. If the shift key is pressed while selecting a configuration, the selected configuration will be appended to the existing configuration.

Pattern Matching

The label extraction option "Property of scan to be used" has the following new choices:
Experiment ID, Humidity, Temperature, and Temperature Difference.

Results Manager

EVA evaluations can be loaded directly from the Results Manager by opening EVA with the database stored data.

Settings

The global setting "Name the document after the first loaded measurement" has been clarified to "Name the document after the first loaded measurement's sample ID or file name". In case the sample ID is empty, the file name is used.

Bug Fixes

- FB#8815: Print preview empty
- FB#8892: View un-grouping leaves views empty
- FB#9296: Scan sample ID entry must be always visible in properties
- FB#9914: PIP and VIP view (and 1D chart copy) contain blank space in Windows 10
- FB#10733: Time decoding for NOUT scans from EIGER detector is wrong
- FB#11171: Export a partial scan of a VDO measurement gives the wrong CPS
- FB#11207: Children Column items are missing in Multiple Properties View
- FB#11455: Area Tool: change of K and Instr. Width is not possible anymore
- FB#11677: Overlay of print objects
- FB#12435: LynxEye properties in integrated 2D detector data
- FB#12488: Sorting in Data Tree does not affect sorting order in Automatic View
- FB#12517: Crash when trying to match non-overlapping scans
- FB#12521: The excluded region is not indicated in Log File View/Report Writer View
- FB#12832: Graphics settings of combined 1D view in print preview were not correctly applied
- FB#12859: hkl generator error
- FB#12886: Pole figure measurements: missing properties (chi values)/wrong display of the x-axis
- FB#12942: X axis in a 2D plot is not correct for measurements with different start values
- FB#12943: Property window empty after right click on the header of a column view
- FB#12958: Absorber and Ni filter not shown in scan properties if they are mounted on the secondary track
- FB#12967: Family parameter in DB browser wrong
- FB#12978: DB/Chemical Filter should not be reset to default as long as the S/M window is open
- FB#13038: Scroll issue with DB view: left part does not show scroll bars when height is reduced
- FB#13039: Phase Sticks not all shown with S/M window open
- FB#13052: By switching to q axis, numbers disappear
- FB#13079: Customization of the 2D View Toolbar is not memorized
- FB#13083: Actualization problem in hkl generator
- FB#13097: Default DB/Chem Filter from Settings is not applied for integrated Frames
- FB#13226: Displacement tool not working with VCT/VSS scan
- FB#13442: Open dialog in DB mode for DQuant and EVA: evaluation name
- FB#13547: Error while closing EVA if it was not completely loaded
- FB#13614: X, Y, and Z drives are not shown for UMC compact stage in EVA v4.3
- FB#13662: Crash when using "Export Scan(s) with Sample ID" and no sample ID is given
- FB#13739: Crash while trying to import a brml which is being measured
- FB#13773: Extended stick view doesn't print nicely
- FB#13836: DB Filter is not applied correctly
- FB#13893: Graphical left x boundary is sometimes zero instead of the lower limit of all scans
- FB#13982: 'Show unexplained areas during S/M' does not work for X-scale d and 1/d units
- FB#14301: Crash during peak insertion near the left side of the diagram
- FB#14389: Wrong French translation for CPS
- FB#14397: GDB file deletion after license expiration fails
- FB#14434: Missing property pane update if "Replace" is called from a tool
- FB#14501: The hkl generator does not take extinction rules into account
- FB#14518: EVA V4.3 crashes after Peak Search Append command if a peak is found at the scan boundaries
- FB#14676: Merge algorithm used for integrated frame merge differs from scan merge in EVA V4.3

VERSION 4.3.2

Bug Fix

- FB#12859: hkl generator error (V4.3.2.1)
- FB#13466: Problem with background tool and curvature 0 (V4.3.2.2)
- FB#13739: Crash while trying to import a brml which is being measured (V4.3.2.1)
- FB#13796: Problem with Y Offset tool for very small offsets (V4.3.2.2)

VERSION 4.3.1

Bug Fix

- FB#13442: Open dialog in DB mode for DQuant and EVA: evaluation name

VERSION 4.3

User Manual and Tutorial

The additions and changes that occurred after print are described in the "DIFFRAC.EVA Manual Addendum" which can be accessed from the start menu or DIFFRAC.EVA's help menu.

New Features

Search/Match (all license levels)

- The user interface for Search/Match has been completely reworked. The tool window is much smaller and the resulting search list is located in the area for automatic views. The search list has been graphically enhanced with icons and colored fields.
- The Search results as well as all filter settings are now part of the scan's memory. This allows going back quickly to former search results just by selecting the scan node without repeating the search.
- The chemical and database filters have their tool windows. This makes working with them more flexible and allows editing filters directly from the scan or the Settings dialog.
- The search performance was improved. A speed gain of up to 30% can be expected, depending on the settings. Repeated searches without filter change are much faster.
- The search result can be sorted by any column, even if the results list contains thousands of entries.
- About 20 new search criteria (sub-sets) have been added to the database filter: e.g. clay, pharmaceutical, SQ-related, and crystallographic criteria
- The sub-sets are grouped according to their relationship given in the search database.
- A switchable lambda cursor allows identifying spurious lines like K_β and spurious W L lines.
- The DB View displays the card status and the ambient/non-ambient status.
- MTC files of DIFFRAC*plus* EVA can be converted into search lists as described in the FAQ document.

Automatic Views (all license levels)

- Depending on the selection in the tree, a range of useful views (mostly tables) is automatically displayed. This feature allows quick overviews of the data's properties.
- A double click on the automatic view tab opens a regular view for later inspection or printing.
- A new setting "Disable some Auto Views (for some 32-bit computers)" was introduced to allow switching off the automatic views for memory-limited systems.

2D Frame Properties (license level V3)

- DIFFRAC.EVA V4.3 support EIGER2 data fully (1D scans, 2D frames, continuous mode, VDO).
- The following properties were added for EIGER2: "Detector Orientation", "Detector ROI 2Theta", and "Detector ROI Gamma".
- In case a measurement has been carried out with variable detector opening (VDO), the relevant properties are displayed as well.

Improvements and Changes

Tool Behavior

- A tool like "Background" stays open as long as compatible data are selected. This was added for convenience to avoid reopening tools for repeated use. Compatible data are data of the same type.

Search List

- The new search list allows fixing the column widths, as requested.

1D View

- There is a new property "Extended View Height" to configure the display. The height is given in % of the main view's height.

DB View

- The card's status is printed (primary, deleted, alternate).
- The non-ambient status is given if it was saved with the card.

Document Properties

- The document has a new property "Data File ID" to reflect the new ID given in V7 (and later) databases. This ID was also added to the list in the "Open from Database" dialog.

Scan Properties

- Starting with EVA V4.3 the Scherrer parameters become part of the scan and cannot be changed individually for single peaks in the Area tool.
- The "PSD Opening" properties for VDO scans have been renamed to "Detector Opening" because area detectors can also measure in VDO mode.
- Background subtracted scans that were exported in RAW format have a flag inside which allows displaying the background subtracted status in the properties. Search/Match takes care of the already subtracted background.
- If a motorized air-scatter slit was used, the opening in mm is given.
- If a non-ambient chamber was used and there was a waiting time before the measurement started, a "Delay Time" is shown in the scan properties.
- The instrument serial number is displayed in the scan properties, if available (BRML files created with Measurement Center V6 and later).
- The property "Database ID" was renamed to "Job ID" to reflect the name used in the measurement software.

2D Frame Integration

- After a 2D frame integration, the resulting scan could have zero count values at the ends. An implicit trimming had been implemented in version 4.0 (stacked frame integration excluded). The trimming behavior can be controlled in V4.3 with the global setting "Trim zeros after frame integration" on the 2D Frame tab in the Settings dialog. The default is "true" and stacked frames are excluded from the trimming.

Peaks and Peak Lists

- To quickly change the color for all peaks of the parent peak list, peaks, and peak lists can run the "Apply Default Colors" command.

Printing

- Report layouts can be deleted.
- The header/footer variable "SCANx_SCANID" was renamed to "SCANx_JOBID".

Miscellaneous

- The setting "Precompute Filters on disk" for the search database is not used anymore and was removed.

Bug Fixes

- FB#443: Wrong behavior when changing the default database
- FB#1782: Problem with view exported via the clipboard to metafile: patterns are lost after editing the picture
- FB#1859: Wrong text for column combos in undo/audit trail
- FB#2760: If an ICDD database was uninstalled, the remaining GDB files cause a license error during EVA start
- FB#3550: Issues converting VDO scans to RAW
- FB#3610: Eva properties: delay time should be shown
- FB#3706: Allow fixing the column width on the search-match candidate list
- FB#4050: Missing linkage between Eva document and corresponding scans in DB
- FB#4932: Exported raw files do not contain a VDO or NOUT indication
- FB#4978: Percent symbol displayed twice in the legend
- FB#5292: Wrong cursor position for 2D mode in the frame view
- FB#6239: "Element #" in database filter not working
- FB#7060: Gamma integration of multiple Pilatus images not consistent
- FB#7539: Issue with DB/Chem. filter when a DIF/STR is imported into a new document
- FB#7926: Remove white spaces in the formula for column views
- FB#7982: Peaks with visibility=false should be ignored in search/match
- FB#8636: Issues with background for VDO and VCT Data
- FB#8642: Problem with the integration of mergeable 2D Mode frames
- FB#8650: Can't import from the database an unfinished scan
- FB#8819: Search/Match database filter "Element # in Formula" is not taken into account if "Min" is checked
- FB#8960: Line cursor integration into the wrong direction
- FB#9126: Wrong unit for sample rotation
- FB#9503: Export of VDO background causes error message and is not recognized as 2Theta axis
- FB#9687: 'Document id' in Print Preview changed to 'Evaluation id'
- FB#10035: Change of Sample ID must not be possible in Part 11 mode
- FB#10406: The user cannot log into the system with another user name by closing the login dialog with the close icon
- FB#10549: Sort by creation date does not work properly for scan lists
- FB#10579: Database Browser for data import: Filtered Results Browser Details table configuration is saved
- FB#10631: Merging of 2D Frames goes wrong with the feature 'Reduce frame size during import'
- FB#10677: Index out of Range Exception when applying Residue on Patterns with VDO scans as parent
- FB#10686: Non-ambient chamber with z positioning has wrong z position in EVA
- FB#10735: Cursor Preview should stay open when a cursor is added or modified
- FB#10753: Soller slit not displayed
- FB#10810: Save the document to the database should disable the OK button if the fields for name and description are not populated
- FB#10855: Wrong error message when exporting partial scans
- FB#10870: Refresh Mask does not work properly for Stackable Frame List
- FB#10895: View Menu - Missing shortcuts for Data Tree/Property/Command Panel
- FB#10953: Negative Smooth Factor not allowed
- FB#10963: PILATUS/EIGER detectors - Numbers on 2D control are jumbled
- FB#10966: Data Tree column width is not persistent
- FB#10967: Crash after opening measure.mdb
- FB#11209: Crash after a double click in the Label tool's graphic control
- FB#11241: A Zeta axis could be interpreted as Z axis and consequently have wrong properties
- FB#11370: Side View display: Shift of X-Axis description
- FB#11404: Problem merging integrated 1D data from multiple frames with varying measurement times
- FB#11574: Information about the air scatter screen is lost in the integrated frame
- FB#11580: Search/Match crashes, if a flat scan is loaded
- FB#11896: Name the document after the first loaded scan does not work in DB mode
- FB#11907: Ca channel different in raw and brml files
- FB#11917: Eva does not display the File Name specified in Start Jobs
- FB#11923: Missing sample properties for scans loaded for pattern matching

- FB#11924: Project ID is missing in Audit Trail
- FB#11984: Modify Psi plot for 2Theta-Integration and inverse Psi tilt (UMC-1516)
- FB#12031: Cursor integration issue for stacked frames with trimmed zeros
- FB#12071: Displacement does not display an error message for txt/xy files
- FB#12119: Crash for pattern PDF 04-009-3818
- FB#12200: A changed scan description is not reflected in the print

VERSION 4.2.2

User Manual and Tutorial

The user manual and the tutorial have the release level V4.0. The additions and changes since release V4.0 are described in the "DIFFRAC.EVA Manual Addendum" which can be accessed from the start menu or DIFFRAC.EVA's help menu.
Please consult the addendum in case the User Manual or Tutorial does not provide up-to-date information.

Improvements and Changes

- The following scan and frame properties for DEBEN tensile chambers have been implemented: "Target Force", "Target Position", "Force" (measured average), "Position" (measured average), and "Load Cell Mode"

Bug Fixes

- FB#3528: Queries to the XRF database don't work correctly
- FB#5001: Icons / Buttons in the top toolbar do not become active when a related item is selected
- FB#7095: Double 2theta cursor in 2D frame views around 90°
- FB#7320: Integration of a large number of PILATUS frames with a small step between frames is not possible
- FB#8046: Import of multiple 2D experiments messes up mergeable and single frame lists
- FB#8695: Exporting VCT/VSS files incorrectly
- FB#8823: "Time started": the wrong unit displayed in the legend
- FB#9087: Cif file with triclinic crystal system wrongly imported
- FB#9096: Crash reading a brml file
- FB#9100: The printout does not print the sample id, but the method name
- FB#9149: XY files exported with FileExchange are not read correctly
- FB#9150: 1D View print does not print the stick patterns
- FB#9304: [hkl] Generator does not create cell parameters for result pattern
- FB#9305: Cell Density should be visible for imported structures
- FB#9306: [hkl] Generator should work for imported structures
- FB#9454: Automatic merge after integration fails for cursor with a small integration step
- FB#9503: crash if [hkl] generator was opened on a scan node
- FB#9581: Wrong y-boundaries for cps presentation in print
- FB#9590: Add SG information in the data tree
- FB#9600: 2Theta-gamma cursor does not work for asymmetric 2D mode frames
- FB#9657: Re-activate the "Repeat Columns" printing features for column views
- FB#9767: Crash in Create Label Column View fixed
- FB#9913: DIF's caption in the 1D chart is incorrect when sticks were deleted
- FB#9914: PIP and VIP view (and 1D chart copy) contain blank space in Windows 10 print preview
- FB#10156: Frame View of Mergeable Frame List shows wrong 2Th values for PILATUS detectors
- FB#10318: Change of Scale properties from Toolbar should be displayed in 2Theta View properties
- FB#10326: Wrong Ka2 ratio displayed; must be 0.514 instead of 0.5
- FB#10458: Accumulate command does not work for VCT scans
- FB#10498: PIP and VIP are wrongly positioned in print or exported bitmaps if the axis is not 2Theta
- FB#10507: Sample ID should be displayed in print
- FB#10810: Save the document to the database should disable the OK button if the fields for name and description are not populated
- FB#11543: "Sample ID" missing in print

VERSION 4.2.1

User Manual and Tutorial

The user manual and the tutorial have the release level V4.0. The additions and changes since release V4.0 are described in the "DIFFRAC.EVA Manual Addendum" which can be accessed from the start menu or DIFFRAC.EVA's help menu.
Please consult the addendum in case the User Manual or Tutorial does not provide up-to-date information.

Improvements and Changes

- There is a new command for (individual) scans: "Export With Sample ID". It works similarly to the already available command for scan lists.
- The scan property "Time per Step" was renamed to "Total Time/Step" to reflect the difference between the time the step motor is programmed to and the accumulated step time for position-sensitive detectors. The step motor time is now "Time/Step" and is shown only for position-sensitive detectors and the BRML format.
- A change in the default database filter (in Settings) is reflected directly in the next search; the default is always set when the search dialog is opened
- New global settings "Enable Deleted PDF Patterns" and "Enable Alternate PDF Patterns" were added to the database tab in the Settings dialog.
- The check for a valid Kβ wavelength was removed from the "Create Kb Pattern" command. The command can now be used for imported scans that do not provide a Kβ wavelength.
- The database browser dialogs for importing measurements and opening documents have more information about the used experiment (name and ID).
- A document loaded from the database displays its database ID and experiment ID in the properties.
- The default settings value for automatic 1D View creation was increased from 200 to 300 scans.
- The document property "Document Version" was renamed to "Software Version" to avoid ambiguity.
- The printing for 21 CFR Part 11 provides more macros for the header and footer (e.g. for signatures).
- The property window remembers its folding state for data of the same type.

Bug Fixes

- FB#3712: Wrong Y-scale values after replacement of a scan or cloning
- FB#6972: 2D Mode frames: Mismatch of line position in Frame View and integrated scan
- FB#7509: Legend display for multi-range scans changed when the Settings dialog is closed with OK
- FB#7623: Wrong frame import into Eva for multiple runs of mergeable frames
- FB#7753: Create Kb Pattern flashes the tree if applied to multiple patterns
- FB#7795: Error reading STR files that do not contain a crystal structure
- FB#7835: A changed sample id is not taken into account when a scan is exported
- FB#7904: Data merging failed for very large data sets
- FB#7929: Ctrl+I shortcut for Import Scan is missing
- FB#7690: Do not display scan properties if the frame was measured stationary
- FB#7693: A second primary slit is decoded although only one slit is given
- FB#8054: Missing unit cell information in the compiled PDF database for monoclinic and triclinic cells with 90-degree angles
- FB#8118: Improved error message if a file has wrongly a BRML extension
- FB#8126: If the s/m dialog is open, the peak list contains a ghost, and the Make DIF command crashes
- FB#8180: Default DB filter not saved if a default database is selected in the Settings dialog
- FB#8226: Cursor coordinates: 2 different values are shown in properties and the tooltip for gamma
- FB#8230: Anode material missing for raw files
- FB#8232: Candidate list: sorting by % values is not correct
- FB#8233: Print does not honor the "Zoom Always Fit Bottom" property if negative values are present
- FB#8235: If several scans are loaded, the opening of the search/match tool takes too long
- FB#8236: 1D View export to metafile: pattern sticks disappear if ungrouped in other software

- FB#8237: RAW Export: the scan mode is not correctly written
- FB#8239: Ca channel missing for exported RAW files
- FB#8251: Predefined chemical filters should discard elements
- FB#8254: The baseline is not correct for unsorted DIF patterns
- FB#8277: The BRML file type shown in Windows should be DIFFRAC.SUITE Result File, not Experiment File
- FB#8288: If the mask selection changed, the intensity sliders in the 2D Frame View changed without effect on the frame display
- FB#8291: Use Custom Mask as Circle did not always switch the mask display
- FB#8339: VCT Measurement: display the correct binding rectangle after import
- FB#8356: Integration of 2D Mode frames does not work properly for wedge cursors
- FB#8421: VDO data export to XYE format: the error column is wrong
- FB#8469: Eva documents from former DIFFRAC.EVA versions: step size in properties is given wrongly as variable
- FB#8470: Exported VCT data (raw) should be displayed in cps only
- FB#8471: Labels are not copied with the Copy as Metafile/Bitmap commands
- FB#8483: Error message after file export (raw and dif) from old Eva document files
- FB#8495: No entry editing possible for DIF properties like Compound Name, Formula, ...
- FB#8513: The signature reason cannot be printed
- FB#8514: Missing items in Print Preview's Header/Footer
- FB#8540: Hide Shadow function does not work
- FB#8542: Wrong Evaluation ID display in document properties after opening a document from the database (the internal value was OK)
- FB#8558: Scrolling through patterns with the cursor keys in the candidate list slows down considerably when the last line has been reached
- FB#8563: Wrong data points when scans from a merged frame are merged
- FB#8580: Goniometer stage not memorized during RAW import/export

VERSION 4.2

User Manual and Tutorial

The user manual and the tutorial have the release level V4.0. The additions and changes since release V4.0 are described in the "DIFFRAC.EVA Manual Addendum" which can be accessed from the start menu or DIFFRAC.EVA's help menu.
Please consult the addendum in case the User Manual or Tutorial does not provide up-to-date information.

New Features

CIF and STR file import (license level V4)

- CIF (crystallographic interchange file) and STR (TOPAS structure) files can be imported and used as patterns for search/match. Importing copyrighted structures is not allowed. Information is displayed if a copyright is detected.

1D View (license level V4)

- Waterfall mode: an additional diagram (Side View) can be displayed on the right side to visualize dependencies between scan properties - useful for non-ambient and DTA measurements.
- The new Scan property "Side View Line Thickness" allows emphasizing scans in the side view.
- The x-y values of the Side View can be copied to the clipboard for further investigation from the context menu.

1D View (all license levels)

- Labels can be inserted and edited. They can have a bitmap or metafile as a label or background and/or configurable text.
- New property "Print Legend under View" allows printing the legend below the graphics.
- New properties "Max Lines in View" and "Max Columns in Print" were added to control how the legend is displayed and printed.
- New tool buttons: Overview, Waterfall, Side View, and Modify Label have been added to the 1D View toolbar.

2D View (license level V4)

- An additional diagram (Side View) can be displayed on the right side to visualize dependencies between scan properties - useful for non-ambient and DTA measurements.
- The new Scan property "Side View Line Thickness" allows emphasizing scans in the side view.

2D View (all license levels)

- The 2D View has a new configurable toolbar like the 1D View.

2D Frames (license level V3)

- Default integration cursors can be defined for frame lists in the Settings dialog – when a frame list is created, the default cursor is automatically applied.
- If the "Automatic Integration" is checked (Settings dialog, 2D Frame page), the default cursor is automatically integrated.
- Create multi-views (merged, stacked) manually only (Settings dialog, 2D Frame page).
- New frame properties like X-ray optics, scan type, and scan mode were added which are available only when the frame is read using the accompanying BRML file.

- A property "Focus Orientation" was added. It will be displayed if the frames are loaded via their corresponding BRML file.
- Properties defining the detector and the optical setup were added: Divergence Slit, Soller Slit, Air Scatter Slit, and Detector Discriminators. They will be displayed if the frames are loaded via their corresponding BRML file.

Frame View (license level V3)

- The Frame View flip horizontal/vertical properties are now configurable permanently in the Settings dialog.
- The Frame View has a new configurable toolbar like the 1D View.

Cluster Analysis Views general (license level V4)

- All views have a **Copy Bitmap** command in the graphic's context menu. The Dendrogram, Scree Plot, Silhouettes, Fuzzy Clustering, and the Parallel Coordinates Plot views haw also a **Copy Metafile** command.
- All views where data can be selected (Dendrogram, Cell Display, all 3D Plots) have now a **Deselect All** command in the graphic's context menu.

Cluster Analysis Thumbnail View is now Well Plate View (license level V4)

- The Thumbnail View has been renamed to reflect its main usage: displaying scan thumbnails according to their sample positions on a well plate. The thumbnail dimensions, the well plate dimensions, and other properties can be configured in the Settings dialog, Properties tab as Well Plate View properties.
- New features: The well plate view honors the sample position if configured in the settings and displays the scans according to the selection below the thumbnail grid.

Scan (all license levels)

- Properties were added for primary monochromators and other X-ray optics. The "Slits" group was renamed into "Optics".
- A property "Focus Orientation" was added.

Pattern (all license levels)

- Patterns have a new **Create Kb Pattern** command to help identify spurious Kβ peaks.

Automatic Residual Algorithm (all license levels)

- The residue algorithm for patterns has a new automatic mode (which can be activated in the tool). The default FWHM value can be set in the General settings.

Cut, Copy & Paste Between Program Instances (all license levels)

- If DIFFRAC.EVA is started several times, data can be cut, copied, and pasted between the instances in the same way as they can be in one instance.

Documentation

- A step-by-step tutorial to convert DIFFRACplus EVA Match files into DIFFRAC.EVA filters were added to the FAQ.

Improvements and Changes

- The peak search accuracy was improved for better peak position accuracy independent of the chosen FWHM parameter.

- Peak search on data with variable counting time (VCT, VDO) will yield better results than in former versions.
- Scans with many thousand measurement points could slow down the peak search considerably. The speed was therefore improved as well.
- A changed default background was only applied if one scan was imported due to performance reasons. This limit has been changed to ten scans.
- The residue algorithm was improved and takes into account the Kβ contribution, the line broadening with 2-theta, and the FWHM of the scan lines corresponding to the pattern.
- The candidates list's columns in the search/match dialog are not automatically resized anymore.
- When a new document is created, the settings for the search criteria are set to the default values: 2 for search in scans and 3 for search on patterns.
- The scan's and frame's properties do not show a fixed value for Phi if the axis was rotated.
- Scans that were created during a 2D frames integration receive the available frame properties.
- A gamma integration with psi as the resulting axis takes the Omega position into account.
- The print header or footer can now contain the scan's database ID and its experiment file name.
- The File Exchange menu item was removed because it is no longer part of the EVA installation. Please install File Exchange stand-alone from the installation medium (DVD or Brukersupport download).
- The database import dialog displays the measurement method id and the measurement method's creation date in 21 CFR Part 11 mode to easily identify the method used for the measurement.

Bug Fixes

- FB#493: Strange line display after Tune Cell tool was opened
- FB#1621: Missing units in the area and peak column views and some properties
- FB#1624: Print legend (or more) below the scan
- FB#1883: Elements in the chemical filter cannot be multi-selected and set to "Mandatory"
- FB#2215: Print preview displays cluttered y-Axis after switching stick view on
- FB#3156: Scan views are occasionally not filled in the print preview
- FB#3612: PIP view not updated when changing the caption margin of the peaks
- FB#3645: Zoom properties were not updated for the frame view
- FB#3668: Property ordering and filtering issues
- FB#3678: Wrong conversion of a DIFFRAC^{plus} EVA document if 2 scans are contained and one scan has a d scale
- FB#3946: Unwanted selection change after scan deletion
- FB#4168: Strange behavior on a 2D view while mouse clicking (right button)
- FB#4254: Margin display issue in PIP
- FB#4470: Results of addition or subtraction of scans shall neither inherit the Y-offset nor the Y scale factor of any parent
- FB#4471: Imported DIFFRAC^{plus} EVA documents have no legend
- FB#4597: Wrong display of y-axis when cps is default y-scale
- FB#4670: Problem with S/M dialog box after docking/undocking
- FB#4671: Fix for manual residue, which didn't work in some very specific combinations of wavelength and line out of scan domain
- FB#4932: Problem evaluating offset coupled VDO raw files
- FB#5118: Wrong zoom rectangle and CPS not fixed after saving and opening of EVA project
- FB#5174: Opening of an Eva document from DB with VDO data causes a strange change of the y-axis
- FB#5182: Display scans X shifted in the graphic which is opened from the cluster analysis Numerical Results View
- FB#5233: Out of range is not treated during copy/paste
- FB#5235: Copy/Paste between scans measured with different X-axes
- FB#5332: Wrong scan color for Accumulate, Add, and Subtract
- FB#5333: Wrong creation date given to scan created by Accumulate
- FB#5648: The column list configuration context menu crashes for stick lists
- FB#5691: The tree is not redrawn under certain circumstances
- FB#5917: Transport the correct time from the frames into the integrated scans
- FB#5996: Issue with the vertical scrolling of the property panel
- FB#6002: Waterfall display bug if scans are loaded later to the scan list
- FB#6111: Angle Psi in scan properties missing
- FB#6179: Side View improvement for data with only one experimental parameter
- FB#6261: The Y-Scale Factor property is not updated after closing the Y-Scale tool
- FB#6267: DIFFRAC^{plus} EVA documents featuring scans measured with multiple wavelengths are wrongly imported
- FB#6313: "Export All Scans With Same Name..." does not use the sample id as file name
- FB#6314: Goebel mirror and fixed slits are not displayed for twin optics
- FB#6379: No information on rotation in Properties for 2D measurements with LynxEye
- FB#6381: Sometimes no 1D View is created
- FB#6444: Wrong X axis for 1D Still scans with LynxEye at 90deg oriented
- FB#6498: FLIP-STICK rotation is shown as "rotating"
- FB#6498: Integrated 1D scan is missing the rotation property
- FB#6562: DIF file sticks disappear during S/M
- FB#6639: The background parameters are not changed in the scan's properties when the background tool is open
- FB#6668: Grouped 1D view always switches on Overview
- FB#6751: VDO files – y-axis should be CPS only
- FB#6764: Continuous scan and Continuous Scan Exact can be displayed in frame properties
- FB#6781: Wrong frame was excluded from the merge list because the detector distance difference limit was too small
- FB#6782: Report does not contain information about amorphous samples
- FB#6792: Y-axis labels are cluttered in the print preview
- FB#6814: Data Tree flickering during search-match when element concentrations are present

- FB#6830: Wrong sign for angular offset; no offset in RAW files
- FB#6843: Wrong intensity of extended view when y-axis is given in cps
- FB#6845: Check mark synchronization for pattern display (Data Tree/Properties)
- FB#6922: Wrong integration when using Ring Cursor as a mask
- FB#6927: Theta is not available as an x-axis for Rocking Curve integration of Stackable Frame Lists
- FB#7002: 2D Mode: Integration of stackable frames can crash
- FB#7009: NOUT: brml files are not displayed/raw files are not displayed correctly
- FB#7139: The top and bottom properties of a VIP/PIP display the y values wrong
- FB#7180: Toolbars are doubled if toolbars were modified and the language was switched later
- FB#7207: Error loading STR files containing commented-out curly braces
- FB#7227: Reverse Y in 2D View properties does not switch the side view's y-axis
- FB#7258: RAW V1 files measured with Co anode are wrongly assigned a Cu anode
- FB#7259: Files that do not have an anode material (synchrotron radiation) get Cu wrongly assigned
- FB#7261: Saving of files containing non-Part 11 scans should not be possible in EVA
- FB#7265: Display of strange Axis offset after brml export to raw
- FB#7291: Crash when using the residue track bar in the search/match tool
- FB#7296: Too many scans read from the database if a multi-scan measurement was imported
- FB#7315: Sample ID is wrongly assigned to Method Name for V2 BRML files
- FB#7324: Pattern height adjustment is not possible for the currently selected pattern when the s/m tool is open
- FB#7344: Display the second primary slit in the scan properties
- FB#7351: Scan sort stripped/unstripped was broken
- FB#7401: 2Theta relative measurements are converted to 2Theta during import
- FB#7550: Divergence slit not displayed after brml import
- FB#7572: S/M on integrated 2D mode frame crashes due to counts below one

VERSION 4.1.1

New Features

2D View

- Background subtracted data can be displayed by checking the property "Background Subtracted".

Document Log View

- The column information is preserved.

Scan Properties

- Kβ filter added

Printing

- Several parts can be printed on one page if they fit. Use the "Can share page" check in the parts table in the Print Preview.

Miscellaneous

- The Ctrl-Tab shortcut key combination was added for fast switching between views.

Changes

- The scan legend default is set to {SAMPLEID}.
- The peak caption is set to {ANG} instead of {INT}.
- The command list remembers its folding state.
- XY files that have no time entry get the time set to 1s (was 'variable').
  It can be changed later in the scan's property window.
- Scan list sorting by File Name and Sample ID added; by Name removed.

Bug Fixes

- FB#1266: Diffrac+ EVA-files are not converted correctly / not at all
- FB#3991: File name gets lost after the reopening of an Eva document from DB
- FB#4405: Change in Dendrogram by "Move Cut Line" will not be shown
- FB#4440: When the 1st scan of a D+ imported EVA document is hidden, many properties of the other objects are wrong
- FB#5241: The silhouettes code failed with a cluster consisting of 2 patterns that are identical in the region 20-60 degrees
- FB#5295: Merge as Single Scan does not work with stacked frames and multiple integrations
- FB#5296: Issue with Grouped View containing Frame View and Frame Header
- FB#5307: Issue with auto Search/Match and tutorial example
- FB#5327: A scan default's description text is missing for the Background Scan property
- FB#5379: DIFFRAC.EVA does not display scans with the type "Still"
- FB#5414: Remove "grey all" and "show selected patterns below" from context menus for views and other tree items
- FB#5415: Move with cursor/selection with the mouse in column views does not sync correctly with the data tree and scan view
- FB#5420: Copy/paste from one edit field to another in the property windows does not work correctly
- FB#5393: Phi and Chi drive positions of a compact stage are not displayed
- FB#5394: RAW file displays a method name although no method is given in the file
- FB#5395: The sample id is wrongly displayed as the method name property for BRML files

- FB#5442: Saving of EVA projects or loading of invalid files results in invisible properties display
- FB#5467: The anti-scatter screen is not correctly displayed in V4.1
- FB#5476: Measurement IDs are lost after saving and reopening a project from the database
- FB#5489: The source database in the DB View sub-file tab was not correctly decoded
- FB#5490: If neither a fixed nor a variable slit was given in a brml file, the DB View did not display any intensity column
- FB#5500: Fixed slits in V1 BRML files are not recognized
- FB#5571: Crash if the residue tool is used on a pattern in the candidate list which is not inserted in the tree
- FB#5530: Crash of EVA Launcher while opening from Windows Explorer
- FB#5600: Document Log View issues: view column information must be preserved, peak search Ka2 removal was missing
- FB#5642: Custom detector distance overwrites the goniometer distance
- FB#5648: The column list configuration context menu misses custom entries if the column list view was created from the document node
- FB#5678: Crash during smoothing
- FB#5707: Tables had a wrong distance to the paper edge if the margin was not equal to 1.0
- FB#5769: Evaluations can be signed even if the experiment is not signed
- FB#5772: Speed problem in Eva after the creation of a DB View
- FB#5785: Frame integration does not take changes in detector distance or angle into account

VERSION 4.1

New Features

Object manipulation in the tree

- Objects in the tree can be cut, copied, and pasted. They also can be dragged and dropped with the mouse.
- Objects in the tree (scans, patterns, peaks, and areas) can be sorted by different criteria. The sorting is synchronized with the related column views.

1D View

- Several new toolbars were added to the 1D View to speed up operations.
- The toolbars in the 1D view are user configurable.
- The lines for selected patterns in the 1D view can have an extra marker in the ruler area. The new command and toolbar button is "Show Selected Patterns in Ruler".
- A new command and toolbar button is available: "Grey All Except Current Selection".
- The data object's visibility can be toggled by a double click or the space key in the tree.
- The waterfall display has a new property "Hide Shadow".

Frame View

- The Color Palette and Intensity range controls in the Frame View can be switched off (also part of the Settings dialog, tab Properties).
- The frame thumbnail view displays colored thumbnails.
- Copy and Save Image As context menu commands added to the Frame View.
- Zoom properties added to the frame view.

Tables and Column Views

- The current column configurations in column views and dialogs containing tables are automatically saved when the program closes and restored after reopening.

Search/Match and Patterns

- A "Search by Name" command was added for scan objects.
- Selected candidates have a colored background in the search/match dialog.
- Patterns that are displayed while the search/match dialog is open have a new "Minimum auto-scale value" in the settings "General" tab. The default is zero which scales the patterns according to their automatically calculated intensity (as in former versions of the program). If the value is larger, patterns are always displayed with the given minimum or a greater scale factor if the automatic scaling is above this factor.
- Unexplained areas are marked in red below the graphics (configurable in the settings, "General" tab, check box "Show unexplained areas during search/match").
- The FWHM used for the residue calculation can be configured in the settings ("General" tab, "The default value for FWHM Residue").
- Pattern objects have a new property "Concentration Level" which marks them as Major/Minor or Trace. The limits can be configured in the pattern list settings.

Printing

- Grouped views are printed on one page.

Changes

- The command "Create 1D View" creates only one 1D view for a selection of objects if they are compatible. Otherwise, only the necessary different 1D views are created (e.g. for different scan axes). The former behavior of creating an individual 1D View per object can be forced by holding the Shift key when clicking the "Create 1D View" command.
- The anode property was switchable for loaded scans that did not have wavelength data. This is no longer possible. The anode and the wavelengths were therefore made available in the Settings dialog, "Properties" tab, object "Scan". The wavelengths can be freely entered.
- The 2D frame integration cursors have larger step sizes of up to 5°.
- The name "Mask" in Cluster Analysis was changed to "Excluded Region".

Bug Fixes

- FB#1396: "Overview" in 1D View is not localized
- FB#2492: The goniometer radius showed the detector distance (frame properties)
- FB#2851: Performance issues if the properties of multiple scans are merged
- FB#3873: The wavelength is not correctly assigned after importing xy data into a scan list with Q axis display
- FB#4023: Export scan to RAW conversion issues: detector data conversion improved, slit unit (°) removed during reading because it could also be mm if converted from
- FB#4181: Pdf export of print preview was missing
- FB#4193: Different results in Fuzzy Clustering View and Log File View
- FB#4205: Not possible to create an area when the x-axis is in d
- FB#4259: The frame thumbnail view is never enlarged
- FB#4301: Scans with anode set to 'Sync' cannot be correctly exported to .raw format
- FB#4304: View update after wavelength change
- FB#4308: A "Compute Crystallinity" property set in the settings causes subsequent file read errors
- FB#4342: Remove leading and trailing zeros from scans resulting from frame integration
- FB#4365: A frame cursor was reset after opening the print preview
- FB#4384: Periodical table in the Chemical Filter tab (S/M dialog box) a has black background
- FB#4390: Change of integration area for Full Frame Cursor should not be possible
- FB#4464: Tooltips in cluster analysis text views added
- FB#4486: Dendrogram View: Silhouettes are missing
- FB#4590: 'Use As Mask' should not appear in Full Frame Cursor properties.
- FB#4672: The hkl generator gives wrong intensities in case of scans displayed with variable slits
- FB#4727: Scan axis after frame integration and scan export is now 2 Theta
- FB#4748: A fixed anti-scatter slit should not overwrite the variable slit flag
- FB#4944: DSRD Compiler issue with French localization
- FB#5017: Files that were opened using drag & drop are not added to the MRU files list
- FB#5018: Reading EVA files with Japanese characters in file names result in an exception "Illegal characters in path"
- FB#5114: Auto-repeat measurement from Commander: time per step is not correct
- FB#5130: A view group should have a "View is Printable" action
- FB#5166: Wrong wavelength for 2Theta frame integration of non-Cu measurements
- FB#5177: A pattern (25-1133) is wrongly named "Quartz" in DB View
- FB#5199: The MDM (most disagreeing member) was renamed to LRM (least representative member) in the cluster analysis 3D views
- FB#5240: For certain data sets the cut level was incorrectly calculated.
- FB#5241: The silhouettes code failed with a cluster consisting of 2 patterns
- FB#5247: Creating a 2D View should be disabled if only a single scan is loaded
- FB#5253: Panning by moving the zoomed area in the overview results in an unwanted view switch
- FB#5259: Forbid "Export Background Corrected Scan" for background scans
- FB#5264: Wrong legend of pie chart in Print Preview
- FB#5265: Change of font size for pattern column view does not work for the printing of grouped views
- FB#5277: Stick children of a DIF were not removed from the 1D View after they were deleted from the tree
- FB#5278: The explanation area below the property control does not display the title text
- FB#5280: DB View: the Ifix/Ivar column moved after switching between fixed and variable slits

VERSION 4.0

New Features

Cluster Analysis (license level V4)

- New commands and views added for cluster analysis; for a description see the "Cluster Analysis Manual"

Miscellaneous (all license levels)

- Tools menu with new commands to start AbsorbDX, FileExchange, and the DSRD Compiler.
- Save As button added to the toolbar
- Export Scan With Identifier command added which uses the scan name as the file name
- Clipboard copy added to 2D view
- Chemical and Database Filter import command added to the respective filters
- Multiple chemical and database filters can be imported at once
- Several chemical filters are pre-installed in the DSRD folder
- [hkl] generator command added to the document node
- Different layouts and settings can be saved and re-loaded (Tools menu)
- Manuals can be displayed directly from the Help menu.
- Experiment added to scan properties for brml files
- AluBath measurements in brml format can be loaded
- The scan property filename will display the database id in brackets if loaded from the database
- New document property: document version
- Lists numbering starts with #1 after a new document was created
- New General settings:
    - Create 1D view automatically for up to n scans
    - Name the document after the first loaded measurement
    - Hide Cluster Analysis node

Changes

- EVA starts by default with an empty document

Bug Fixes

- FB#1387: Empty Print Preview
- FB#1840: Issues with the Kb images of a pattern
- FB#2243: Minor issue with the installation folder of COD
- FB#2733: CHC chamber: wrong category for humidity measurement
- FB#2998: Append a scan with a y-offset and get twice the scan with the offset
- FB#3061: Error while importing a D+ document with given attributes.
- FB#3102: The coloring in the waterfall view did not work for background-subtracted scans
- FB#3132: Text missing in the hkl generator when using the BrukerBlue skin
- FB#3416: Error during experiment import from database "Error while opening ...: Illegal characters in path."
- FB#3499: "Scan 1 Operator" is not filled in the printed header or footer
- FB#3692: Global Area Column List does not use the correct column configuration
- FB#3712: Wrong Y-scale values after replacement of a scan or cloning
- FB#3747: Reproducible crash with a given document
- FB#3773: Periodic table entry Pa is wrongly displayed as Palladium.
- FB#3775: Scan View is not updated if the underlying scan is modified
- FB#3838: a/c value in DB View was inverted
- FB#3880: Extremely slow New action with EVA documents containing many column views
- FB#3883: User patterns created from scans measured with variable slits have wrong relative intensities

- FB#3909: Peak search bug fixed which degraded the algorithm in V3.2
- FB#3943: Missing unit in legends
- FB#3946: Unwanted selection change after scan deletion
- FB#3949: The label variables for heating rate and temperature differences are wrong
- FB#3969: Property grid title for multiple properties shows the name of the first selected data item
- FB#4011: A 2D view crashed during printing
- FB#4036: Unzoom issue for CPS scale
- FB#4039: Crash in DSRD Compiler if a user database folder was selected which did not contain a user database
- FB#4063: Cumulative Y-scale-factors combined with cumulative Y-offsets issue
- FB#4131: Crash in the database browser dialog if Measurement.mdb contains user-entered fixed compounds
- FB#4194: Wrong temperature displayed for brml files (file version 3.3.35)

VERSION 3.2

New Features

2D Frame Data (license level V3)

- 2D mode frames can be imported and integrated
- Integration into a Psi-scan for wedge cursors
- The intensity slider control and the color palette in the frame view can be switched off
- Open a single frame view automatically for every loaded frame or every loaded single frame; this is configurable in the Settings dialog
- Custom detector center is a real number point instead of an integer

Miscellaneous (all license levels)

- The new VOD data can be opened and displayed; related properties are added to the scan; the default background is "Enhanced" and has a curvature of 0.02
- Command "Export Background Subtracted Scan" added
- Command "Accumulate" added for scans
- "Sum" added to the frame view's "Display" property for stacked frames
- Scan mode, sample position, measurement duration, and heating rate added to scan properties for brml files
- Different primary and secondary track radii are displayed
- Index column in Scan View; columns can be sorted and exported to the clipboard
- Columns in the search/match tool, candidate list can be sorted
- Units are displayed and printed in the column views
- Allow adjusting the number of decimals for the SQ% parameter (Settings dialog)
- The Tune Cell tool allows selecting hk0 for tetragonal and hexagonal crystal systems
- Scan fill color property for the 1D waterfall view which hides hidden lines
- Some default table configurations have been added to the column views
- Table printing options added: fit columns in one row, distribute columns on several rows, auto size
- Table printing options are saved in the document and available as default properties (Settings dialog)
- The font for the DB View printout can be changed.
- "General" page added to the Settings dialog with a field for the default print layout and the graphics export bitmap size
- Possibility to define columns for database browser (Import from Database and Document Open)
- EVA files are always compressed and the former separate EVA.BIN files are part of the archive
- The recently open document is re-loaded after a language change
- The User Manual and the Tutorial will be displayed in an internal viewer – no external PDF viewer is required
- DIFFRAC^{plus} user databases can be converted with the DSRD Compiler
- The installer program for the Crystallographic Open Database (COD) has been updated to support the new version

Changes

- 2D frame loading, display, and integration performance improved
- The start menu shortcut "DIFFRAC.EVA" starts the program in a file-only mode. The new shortcut "DIFFRAC.EVA (database access)" provides additional access to the measurement database and requires a login.
- If EVA is started without a database connection (the default) the title bar shows "no user logged in" instead of the misleading "EvaluationUser"
- EVA file format updated

Bug Fixes

- FB#920: The bottom slider below the frame does not show the min and max values.
- FB#1010: A detector axis as a scan axis does not allow Search/Match for brml V3 data
- FB#1095: When printed as PDF the pie chart is not printed
- FB#1185: The image exported from Print Preview has a black frame
- FB#1381: Problem with integration when some parts of a merged frame do not contribute
- FB#1435: If the Print Preview is opened with a selected document and the print layout is changed the document's layout is not updated
- FB#1462: Missing feature in the background tool: "Original measurement"
- FB#1799: Ctrl+left mouse button for scaling pattern sticks is too slow
- FB#2236: Variable step size after frame integration with area cursor
- FB#2294: Wrong scan Time Started value, if the time difference between the first scan and the actual scan is a day or more
- FB#2312: Index out-of-range exception in xy/y scan export
- FB#2313: The heating rate is displayed instead of the temperature
- FB#2350: Decimal places for 2Theta/Theta angles were taken from the drive and not from theta format
- FB#2368: Wrong unit for LynxEye 0D opening
- FB#2411: Crash during DIFFRACplus EVA document import
- FB#2676: Space groups not displayed for COD patterns in search/match candidate list
- FB#2726: Show phi oscillation amplitude and speed for frames
- FB#2717: Display the corrected sum count instead of the raw sum count in the frame properties
- FB#2768: Wrong phi-oscillation speed for raw files (0D mode)
- FB#2774: Brml file reading problem with French EVA
- FB#2766: Missing property update if the waterfall view's offsets were changed using the scroll bars
- FB#2806: Message "No experiments found in database" even if the Cancel button was clicked
- FB#2853: Incorrect detector opening for LynxEye 0D
- FB#2867: Incorrect oscillation speed for raw files
- FB#2872: Crash during startup if the license server is missing
- FB#2880: Waterfall view: x/y offset should be persistent
- FB#2899: Discriminator values are not displayed for brml files measured with 1D detectors
- FB#2928: An anti-scatter slit was displayed as a detector slit
- FB#2932: Detector slit not displayed correctly
- FB#2965: Import of xye-files does not read the error column
- FB#2998: Append a scan with a y-offset and get twice the scan with the offset
- FB#3022: Incorrect step size for VCT raw files
- FB#3017: Missing Creation Date/Time for integrated scans from GADDS frames
- FB#3070: Detector opening unit missing in raw files
- FB#3092: The slit units were sometimes wrong for raw format files
- FB#3100: Discrepancy in the number of lines between the DB printout and the stick column list
- FB#3115: The sorting function in columns containing a number at the end does not work properly
- FB#3143: Discriminator width added for scintillation counters
- FB#3153: Rotation speed for Phi scans (0D) not shown if zero
- FB#3208: Partially measured scans were not displayed
- FB#3261: Stick deletion is too slow
- FB#3265: The pie chart disappears as soon as a DIF is added to the scan list
- FB#3269: Print Layout is not saved with Eva document
- FB#3271: Wrong results for areas from scans with Y-offset and Y-scale applied; old EVA files will still show the same bug as it is directly connected to how areas are stored in the EVA file
- FB#3329: Area tool graphics error with BG and slit simulation
- FB#3331: 2D view reset (zoom, color level) changing a 2D view property
- FB#3356: DIF created on a scan measured with variable slits is wrongly scaled
- FB#3363: Impossible to normalize two data sets if one has a simulated slit mode
- FB#3372: S/M candidates containing a delta in the name were not properly filtered
- FB#3491: A DIF file was loaded using Cu for d-2Theta conversion even for scans with different wavelength
- FB#3501: An installed DSRD database is not found by EVA (SQLite error)
- FB#3502: Numbers in curly braces are shown in tooltips for the property grid and tree
- FB#3552: A single scan with all zero y values is not displayed in the 1D View
- FB#3576: Area not properly displayed on background subtracted (display) data

- FB#3579: Scan end property for unfinished scans should be adjusted to the last measured x position
- FB#3676: Error message when closing Import files dialog with Cancel after Clone or Replace

VERSION 3.1

New Features

2D Frame Data (license level V3)

- Integration cursors can be exported and imported
- Option to reduce frame size by a factor of four during import in the Settings dialog

Miscellaneous (all license levels)

- Ca channel measurement time added to the scan properties
- Temperature difference added to scan properties for DTA measurements
- PDF-2 and PDF-4 Release 2013 and PDF-4 Organics Release 2014 are supported
- Crystallographic Open Database (COD) was updated to REV89244 (2013/10/11)

Bug Fixes

- FB#107: Floating panels are not shown after a restart of Eva. The error is "Problem while reading current Layout". Remark: floating panels may be displayed behind the main window after reloading. Loading data or switching the program's window state will make them reappear.
- FB#109: If a user database consists of DIFs that contain no formula the search match fails
- FB#484: Raw or brml files are not visible after import in Eva on slow computers
- FB#487: VCT measurements in Eva: force CPS display and do not allow counts in the 1D view
- FB#879: The memory consumption is very high for multi-range files
- FB#1451:Issue with copy/paste of numerical values larger than 999
- FB#1456:Some RAW files with coupled 2Theta/Theta axis are loaded into an AUX scan list
- FB#1461:"Ghost" for Y-Offset is not displayed correctly when applying the correction more than one time. The same fix applies to X-Offset and the Y-Scale.
- FB#1463:Crash in merge algorithm for non-overlapping scans
- FB#1464:Negative intensities after merge
- FB#1470:Exporting multiple scans from a scan list does not honor background correction or slit simulation
- FB#1473:Memory leak in RAW file reader
- FB#1491:Patterns shown for variable slits are scaled for fixed slits
- FB#1497:Temperature is always given in °C even if Kelvin was given in the measurement
- FB#1529:Acrobat Reader does not start on Windows Embedded operating systems (D2 PHASER)
- FB#1580:Pattern context menu in the Candidate List is not displayed
- FB#1601:Background tool is slow for multiple selections
- FB#1706:Issue with the selection within the "selected candidates" list
- FB#1783:Raw files exported from brml files with 2Theta scan-axis (PSD fixed) are imported into an Aux scan list
- FB#1802:Wrong divergence slit unit
- FB#1812:Frame integration minimum is set to 0.1 degrees
- FB#1909:PDF card printout restriction of 276 lines removed
- FB#1956 HKL Generator: Parsing bug for comma decimal separators fixed
- FB#1984:Prevent frames to be merged if they were measured at different sample positions
- FB#2025:Crash after opening the Y-Scale tool and clicking on the "Extended" scan property
- FB#2096:1D View: the logarithmic scale's lower limit was 10 cps, which is now 0.01 cps
- FB#2104:Printing: the DB View's d-I table repeats its last line in the next table if the table is split
- FB#2188:A fixed secondary slit overwrites a variable primary slit

VERSION 3.0

New Features

2D Frame Data (license level V3)

- 2D frame data can be loaded, displayed, integrated, and printed
- Single frame integration over Gamma and 2Theta with full frame, wedge, ring, and line cursor
- Integration on merged frames with slice, wedge, and ring cursor
- Multiple integrations on stackable frames with one click
- User-configurable masks with angular or pixel coordinates
- "Rocking curve analysis" on stackable frames with various frame properties
- Frames are automatically grouped into mergeable or stackable lists
- For large zoom factors the 2D view displays count numbers inside the pixel areas

Miscellaneous (all license levels)

- The view tree was merged into the data tree and an automatic view filtering dependent on the data selection was introduced
- Properties can be filtered and grouped or ordered alphabetically
- An hkl generator is available for scans and patterns
- Scans in xy format can be imported and exported; the anode material for such scans is selectable
- Scan lists can be exported as multi-range files or as individual files at once
- A Scan View was added to display X-Y-Time values
- A print can contain user-configured document and measurement data property values in the header or footer
- Exported scan files have "exported" and if requested the angular range in the file name
- AbsorbDX program added
- Chinese translation added
- A color legend and a reset button were added to the chemical filter tab in the Search/Match dialog
- New global setting in the Settings dialog, Properties tab: Automatic multiple properties display
- New data properties:
  Document: Print Layout, Creation User, Last Write User
  Scan: Creation Date/Time, Last Write Date/Time, User Comment
- New view properties:
  1D View: Print Width, Print Height, Waterfall Offset X, Waterfall Offset Y
  Chart View: Font
- New default properties:
  Scan: Background properties
  Pattern: Caption

Changes

- FB#66: No user-dependent data are created during installation. The first time EVA run starts loading these data from the application data folder.
- FB#68: Change the defaults for the 2D colors to "Rainbow".
- FB#83: The 2D frames are loaded from the brml references. There are unified Import commands to import the data from the file system or the database.
- FB#94: Display the "tuned" information for patterns in the data tree to avoid errors.
- FB#97: Provide properties for the waterfall plot: X and Y translation
- FB#102: The pattern's quality mark is displayed in the properties.
- FB#103: The pattern's Caption property is available in the Settings dialog.
- FB#104: All documents are copied to the installation folder and are accessible from the start menu
- FB#110: Auto scale issue for y-axis after replacing a scan
- FB#144: Loading speed improvement by pre-compiling during installation
- FB#147: If a scan has a simulated slit (variable or fixed) the simulated data are exported with the "Export Scan" command.

- FB#224: The view tree was merged into the data tree. The panels belonging to the view tree were removed (View Command, View Tree, and View Properties)
- FB#228: The strict operating prerequisites (Windows XP 32bit and Windows 7) were lifted in the installation software. It is possible to install the software on other operating systems at the user's risk.
- FB#235: The lattice parameters were added to the search/match candidates list.
- FB#301: The COD2011, COD2012 and COD2013 can be installed with DIFFRAC.EVA V3.
- FB#390: Reset button added to the chemical filter dialog page
- FB#393: Usage period for evaluation licenses added to the About dialog
- FB#398: Color legend added to the chemical filter dialog page
- FB#439: The report layout is now stored in the EVA document.
- FB#156: The license level is displayed on the About dialog's general page.
- FB#652: An automatic Apply is triggered when Print is clicked in the Print Preview
- FB#876: Multiple selected files which are opened from the Explorer start only one EVA instance.
- FB#917: A background subtracted scan is saved if the display is set to background subtracted.
- FB#1290:Tune Cell did not take peaks with less the 5% intensity into account, the limit is now 1%
- FB#1373:The minimum and recommended hardware requirements were modified to avoid situations with extremely slow operation.

Bug Fixes

- FB#112: The database filter table in the Search/Match tool is not translated
- FB#115: There is no unit displayed for motorized slits if they are set to fixed opening
- FB#122: Using the legend does not work on some postscript printers/pdf creators
- FB#135: Print Preview does not display scroll bars
- FB#136: Pattern sticks display the wrong tooltip
- FB#141: Issue with scaling of VIP for a y-scale in cps
- FB#142: Wrong intensity after normalization and application of y-scale factor for y- scale in cps
- FB#146: Intensity problem after simulation of slit mode
- FB#223: No question to save a changed project is asked if another project is loaded via the MRU list
- FB#242: During uninstallation the start menu items were not removed.
- FB#347: Crash after switching from cps to counts
- FB#301: COD's EVA version detection prevents installing COD on computers where only V3 is installed
- FB#380: Cannot load certain HighRes brml files created with MC V2.2.66
- FB#383: The palette colors in the 2D view display the wrong colors for the logarithmic scale
- FB#384: A language change could change the number format
- FB#458: A change of pattern intensity scaling should be visible immediately in properties
- FB#483: Missing properties for raw and brml files
- FB#586: Crash if a command in the command bar was hit after deleting the referring data object
- FB#589: Import from XRF database in pre S+ V3 format is extremely slow
- FB#624: The output in PolySnap views (OpenGL) is scrambled
- FB#838: The chemical filter fails if H is selected blue, grey, or green
- FB#918: Oscillation is not shown in scan properties
- FB#1010:A detector axis as a scan axis does not allow Search/Match
- FB#1023:Wrong display of the Detector Opening Angle scan property if Windows is set to use comma-separated numerical values
- FB#1124:Problem with intensity scaling on EVA files after a change from counts to cps
- FB#1224:Opening many files with drag and drop is very slow
- FB#1360:After a Search/Match the results list is not focused and the keyboard cannot be used to browse the list
- FB#1389:The candidate list becomes blank when removing the pin to enlarge it
- FB#1394:Axis name issue for exporting a TwoTheta scan to raw format
- FB#1395:The background and peak search tool sliders cannot be moved

VERSION 2.1

New Features

- Seamless import of legacy DIFFRAC*plus* EVA documents (see Manual Addendum in the Documents folder, topic "Automatic conversion of DIFFRAC*plus* EVA document files (*.eva)…")
- DIFFRAC.EVA is delivered with the COD2011 database on the installation CD

Changes

- Importing several measurement files containing multiple scans combines all scans with the same axis in one scan list
- Importing a measurement file containing multiple scans from a scan list node inserts the scans into the scan list if the axes match
- New defaults for 1D View: Overview auto hide; Show legend
- New default for a Pattern: Legend {PATT} {FORM} {COMP}
- Improved French translation

Bug Fixes

- RT#7054: After the merge of vct data the resulting measurement time is different for raw and brml
- RT#7085: Intensities in stick view and peak view are different
- RT#7100: The .NET 4.0 installer which is part of the installation program does not report a too-small free disc space
- RT#7112: VIP or PIP button with Residual scan button remain pressed and a scissor is wrongly displayed
- RT#7121: Relative intensity of peaks is negative if the background is high
- RT#7125: Importing RAW2 files that were converted from RD format gave a start angle of zero
- RT#7129: For files with very large step sizes the search/match may crash
- RT#7130: Files with extensions that are not all lowercase cannot be loaded with drag and drop
- RT#7148: The time per step which is displayed for brml files is the planned time, not the measurement time
- RT#7156: The wavelength selection in the DB View does not show the wavelength used for angle calculation
- RT#7168: Print margins in Print Preview are given in inches with a factor of 100
- RT#7170: EVA in the French language cannot open certain brml files
- RT#7364: Problem with wavelength change for PDF cards
- RT#7365: Wrong d and 2Th values in DB view for non-"original" PDF cards
- RT#7376: A crash may occur during the EVA shutdown
- RT#7378: If EVA opens a temporary brml file, the file may not be written properly by the ICS software
- RT#7398: The DSRD compiler reports an error message for PDF-4 when the compilation starts
- RT#7403: wrong intensities in the stick column view after export/import of a dif file
- RT#7405: If a pattern is appended after a tune cell or dmulby action, a view is created from this pattern and the project is saved, the resulting view is linked to the original pattern
- RT#7406: The scan import action misses the internal undo functionality
- RT#7413: The Mo Ka1/2 wavelength in the pattern property window is wrong

VERSION 2.0

New Features

- Automatic search/match algorithm (only available for V2 licenses)
- Compatibility with PDF-4+ 2011, PDF-2 Release 2011, and PDF-4/Organics 2012
- Scans order and reverse order properties for 2D and waterfall view (only available for V2 licenses)
- Tooltip in 2D view which displays the selected scan order parameter (e.g.) temperature; axis descriptions
- "Scan grid" property in 2D views which is helpful if oddly spaced scans are displayed
- "Replace Scan…" and "Clone Scan…" commands accessible from a data scan node
- Shortcut keys for hiding all panels (Shift-F1) and showing only individual panels (Shift-F2…Shift-F7)
- "Export partial scan…" and "Export background…" commands accessible from a data scan node
- Eva, raw, and brml files can be transferred on the command line and opened with a double click
- More measurement properties are displayed: "LynxEye 0D", "Detector opening angle", "Detector slit width", "Primary Soller slit", "Secondary Soller slit", "Sample rotation speed"
- Raw files which contain Ca channel information exhibit a new scan property "Ca Channel" displaying the respective pulse rate
- DIF files can be imported and exported
- New commands for the document's Settings node: Clear Default Filters, Create Chemical/Database Filter Data, File Import Chemical/Database Filter Data
- New commands for the Chemical and Database Filter nodes: Use as default Chemical/Database Filter, Export Chemical/Database Filter

Changes

- Better coloring for the candidate and document phases while the Search/Match tool is used with new properties to control the coloring
- Improved user manual and tutorial
- Improved localization

Bug Fixes

- RT#7119: Pattern intensities were displayed incorrectly in the graphical view for variable slit measurements
- RT#7118: EVA could crash while importing XRF data from measure.mdb
- RT#7115: Problem with the scale factor for VIP in print preview
- RT#7113: The ghost may have disappeared from the search list
- RT#7112: VIP or PIP button with Residual scan button remained pressed
- RT#7107: Grid printing for 1D views
- RT#7106: Raw file export did not export the temperature, humidity, and axis positions
- RT#7105: Crashed when printing
- RT#7103: The dongle driver caused program freezes after hibernation for certain dongle firmware
- RT#7102: Raw export for merged scans was not possible if the resulting scan had a variable step size
- RT#7101: Raw files could not be exported to file names/paths containing Unicode characters like Japanese or Chinese names
- RT#7098: Crashed when merging brml vct data
- RT#7096: Only the first scan of a multi-range brml file could be exported

VERSION 1.4

New Features

- Experiments with GID-Tracks and Bond-Tracks can be evaluated
- Compatibility with DIFFRAC.SUITE measurements (*.brml) up to version 2.2

Bug Fixes

- RT#7082: Scans created with the background or subtract tool were not exported
- RT#7088: Slit openings were not displayed correctly for BRML files

VERSION 1.3

New Features

- General performance improvement
- Compatibility with DIFFRAC.SUITE measurements (*.brml) up to version 2.1
- New color coding to display the data-view connection
- Language switch in the View menu

Changes

- Patterns without valid cells can be inserted into user databases
- More possibilities to label patterns and sticks (PATT, COMP, and FORM)
- For multi-scans, the background is not displayed by default to increase the speed
- Improved localization

Bug Fixes

- RT#7015: Performance: Y-scale in Selected Candidates reacted slowly after applying green filter data from the element list
- RT#7072 Bug: DSRD Compiler was not able to compile PDF-4 2010/Organics

VERSION 1.2

New Features

- French, German, and Japanese translations
- COD Phase Database installer on the CD in the COD sub-folder

Bug Fixes

- RT#7051: Search Match for measurements with short wavelength failed intermittently
- RT#7062: Divergence and anti-scatter slits were interchanged for brml files

VERSION 1.1

New Features

- User Phase Database support
- COD Phase Database support
- PDF2010 and ORG2011 support
- Customizable Database Filters
- View type: Chart View
- Extended View
- Configurable printing options
- Database and Filter Defaults in the Settings dialog
- Windows 7 32bit and 64bit compatibility

Changes

- Patterns can be imported into an empty document without loaded scans
- BRML file import supports DIFFRAC.SUITE Version 2 files

Bug Fixes

- RT#7011: The displacement tool failed to display the shift of an appended scan
- RT#7012: After merging scans, the position of the high angular values was shifted
- RT#7035: Use of PDF4 on D2 required a fix
- RT#7039: Area creation for negative x-values was not possible
- RT#7053: No Ka2 stripping possible on LynxEye equipped D2 instruments

VERSION 1.0

This is the first version of DIFFRAC.EVA.

Appendix – Features, Versions, and License Levels

Feature	Required version (license level)
More precise automatic search/match	V6 (V1)
Automatic displacement correction after search/match	V6 (V1)
Comprehensive, self-compiled COD including crystallographic structures	V6 (V1)
Matching lines view	V6 (V1)
TOPAS project file export	V6 (V6)
Evaluation result export to database	V6 (V6)
Online evaluation for SQUALL and PMI	V6 (V1)
Use of PDF-4+ Web	V5 (V1)
Peak fit	V5 (V5)
Match peak	V5 (V5)
Structure file export	V5 (V5)
Compact scan list for large files with many scans	V5 (V5)
Quantitative analysis with SQUALL (in pattern matching)	V5 (V5)
Positive material identification (PMI in pattern matching)	V5 (V5)
Labels	V4.2 (V1)
Side view	V4.2 (V4)
Structure file import	V4.2 (V4)
Toolbars	V4.1 (V1)
Cluster Analysis	V4 (V4)
Automatic frame integration	V4 (V4)
Saving the workspace layout	V4 (V1)
Saving the EVA settings	V4 (V1)
Support of DIFFRACPlus user databases	V3.2 (V1)
Duplicate scan	V3.2 (V1)

Feature	Required version (license level)
Accumulate	V3.2 (V1)
Export background subtracted scan	V3.2 (V1)
Document log view	V3.1 (V1)
2D frame data loading and display in several view types	V3 (V3)
2D frame data integration	V3 (V3)
2D frame data masking	V3 (V3)
2D frame data rocking curve analysis	V3 (V3)
Hkl generator	V3 (V3)
Property filtering and grouping	V3 (V1)
Scans in xy format	V3 (V1)
Scan view	V3 (V1)
AbsorbDX program	V3 (V1)
Automatic search/match	V2 (V2)
Export partial scan	V2 (V1)
Export background	V2 (V1)
Replace scan	V2 (V1)
Clone scan	V2 (V1)
Database and chemical filter commands	V2 (V1)
Scans order	V2 (V2)
Shortcut keys for panels	V2 (V1)
Automatic conversion of DIFFRAC*plus* EVA document files (*.eva) into DIFFRAC.EVA document files	V2 (V1)