

Bruker XRD Diffrac.EVA Quick Start Guide

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Introduction

This guide is a quick introduction to the DIFFRAC.EVA software (version 5.1) and how to use the program to solve crystalline phase identification. For detailed information and an in-depth guide refer to DIFFRAC.EVALUATION User Guide & Tutorial available in hard copy in the X-Ray Lab or online in Cumulus at [XRD Books and Reference Material](#).

For former version of DIFFRAC.EVA software, refer to hard copy available in the X-Ray Lab.

Opening a Diffractogram in DIFFRAC.EVA

To open a diffractogram for evaluation:

Click **File > Import from Files** (*Figure 1*). Select the file you want to open. The D4 Bruker scans are saved in C:\DATA\IN. Click **Open**. The scan is now open and ready for evaluation. DIFFRAC.Eva can open/import files produced by both the Bruker and the Aeris XRD in the x-ray lab. The valid formats are .raw (Bruker) and .xy (Aeris, see the [Aeris Advanced User Guide](#) for instructions to convert .xrxml files to .xy files). It is also possible to analyze Bruker scans with the Aeris HighScore Plus software, which can open both .raw and .uxd files without conversion.

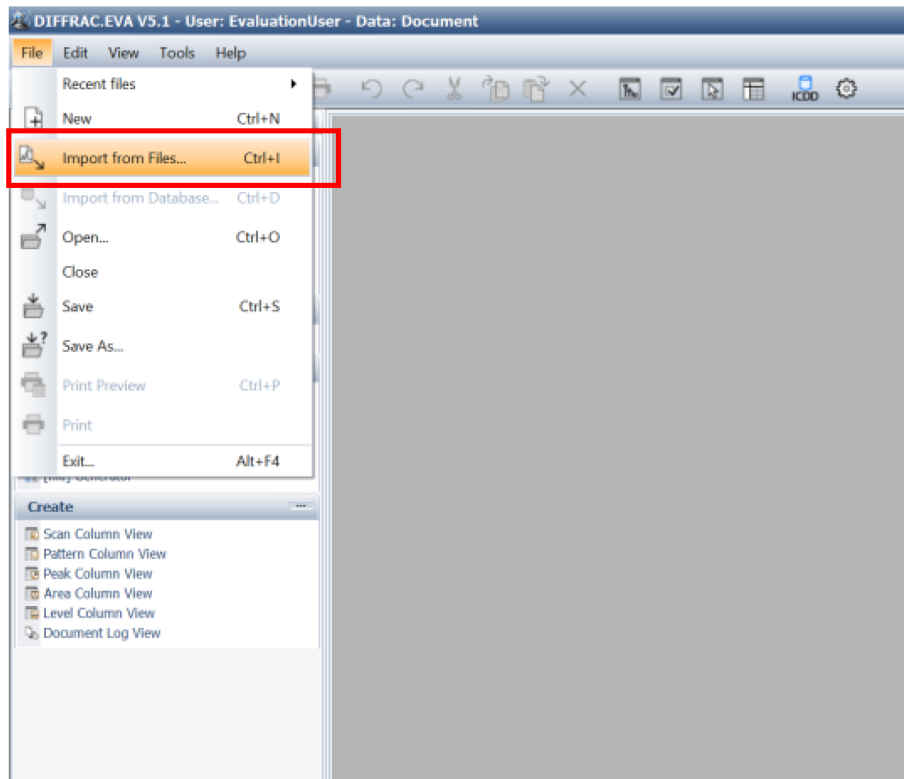


Figure 1. Open Scan.

The DIFFRAC.EVA main screen has the following primary functional area (Figure 2): a **Toolbar**, a **Data Command Panel**, a **View Window**, a **Data Tree Panel**, and a **Data Property Panel**. An additional window, called 'Automatic Views Panel' can be open by clicking **View > Automatic Views Panel** in the top menu.

It is useful to have the **Data Command Panel** and **Data Tree Panel** open for view at all times. Use the icons in the **Toolbar** to open/close these views.

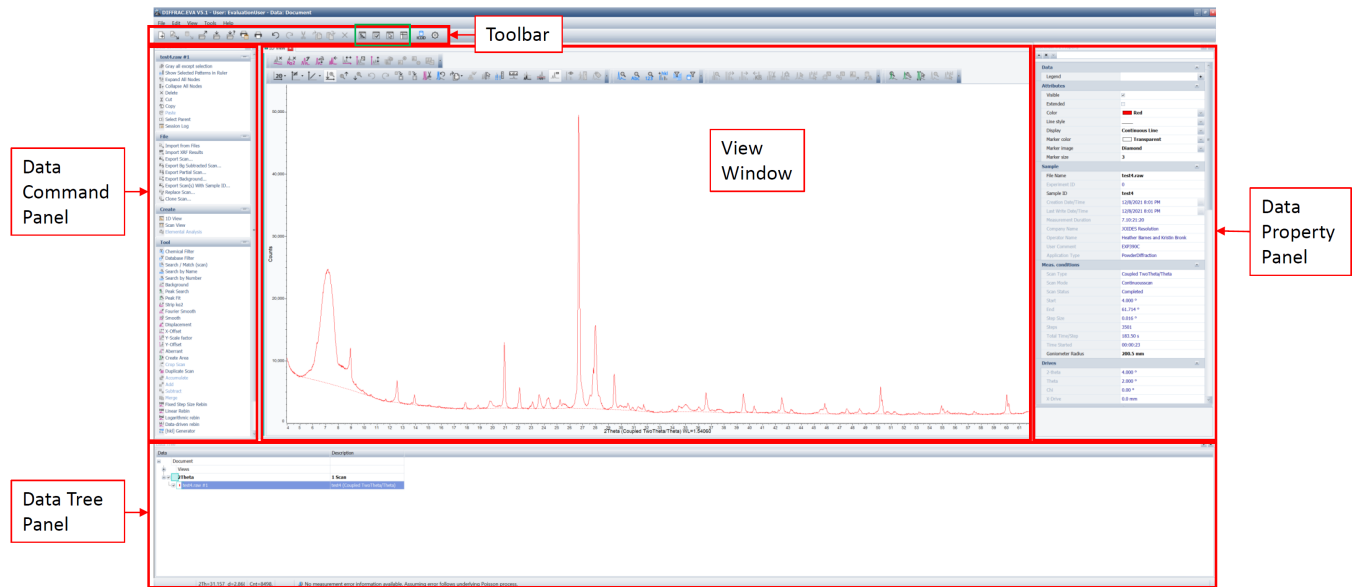


Figure 2. View of a Diffractogram in EVA

Removing the Background

The first step in preparing a scan for Search/Match phase identification is to subtract the background (Figure 3). There are two methods for removing the background:

- **Traditional method:** is recommended for all scans; it gives an arc parabola but never submerges a complete peak.
- **Enhanced method:** gives a smooth curve where some peaks may be under the background curve. This could be useful for crystallographic studies. See the EVA manual for greater detail.

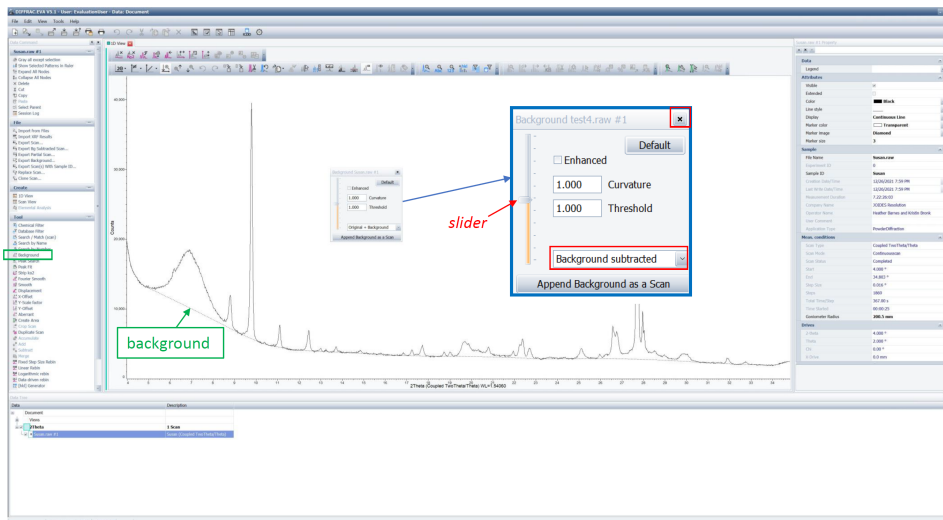



Figure 3. Background Highlighted in a Diffractogram and Background Dialog Box in inset

In **Data Command Panel**, select **Tools > Background** to open the Background dialog box (Figure 3). Default view is 'Original + Background'. If needed, use the slider on the left to adjust the curvature on background humps. When satisfied, in the drop-down box, select **Background subtracted** option.

Close the text box . The background is removed, and the diffractogram is changed to baseline.

Search/Match

The **Search/Match (scan)** tool in the **Data Command Panel** attempts to match XRD scans with patterns found in the ICDD (International Centre for Diffraction Data) PDF database. The Search/Match process tries to identify an unknown scan based on pattern recognition techniques. EVA can also find a reference pattern by its name or ICDD number.

Note: It is at the user's discretion to identify and choose the correct pattern matches.

In **Data Command Panel > Tool**, select **Search/Match (scan)** (Figure 4A). 'Auto Views Panel' pops up if not open yet (Figure 4B). Notice the Search/Match dialog box has four tabs (Figure 4C):

- **Databases** : includes DB Filter and Chemical
- **Match Lists**
- **Names**
- **Options**

Select the desired search parameters (see suggestions below and Figures 6, 7 and 8).

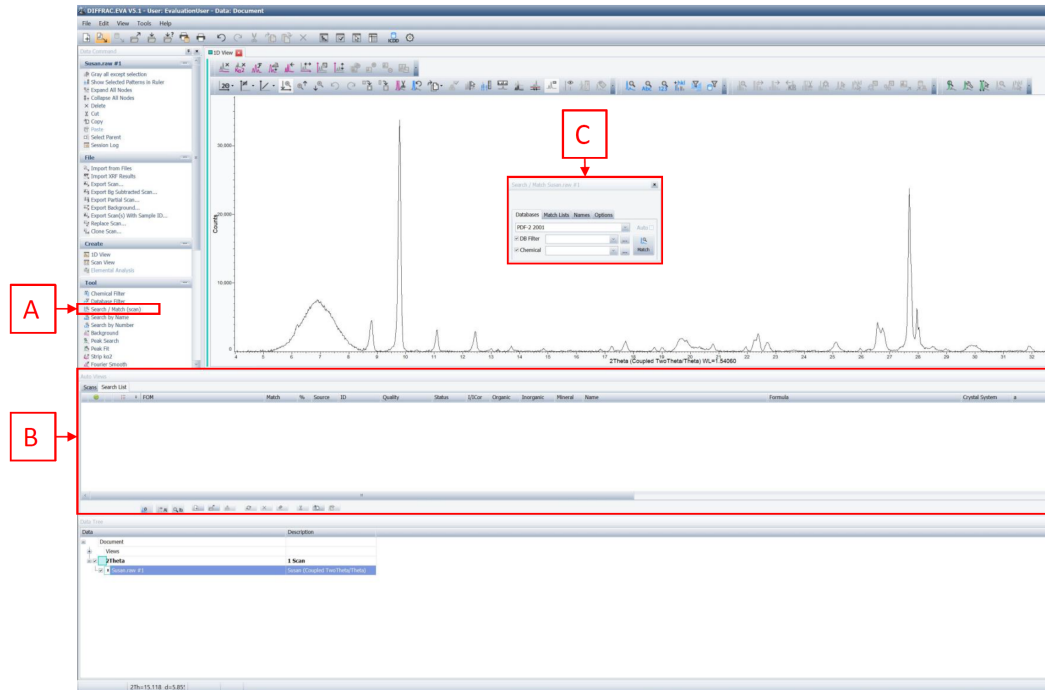


Figure 4. A. Search/Match, B. Auto Views Panel, C. Search/Match dialog box

In the **Criterion** field of the **Options** Tab (Figure 5), begin the search with **2: Neutral**.



Figure 5. Options Tab of Search/Match dialog box.

Database Filter

In the **Databases** Tab, select the **DB Filter**. Click on the "three dots" button (Figure 6A). The Database Filter window opens (Figure 6). The default name is 'Database Filter #1', and the database used is "PDF-2 2001". The Search/Match can be enhanced using database filters such as the following (Figure 6):

- Quality Marks:** Degrees of pattern quality assigned by ICDD. Recommended: *, Calculated, Indexed (a).
- Status:** Recommended: Primary (b).
- Colors:** Select the color of the mineral to be searched.
- Sources:** Database section: select both ICDD Database (experimental) and ICSD Database (ICSD-FIZ) (c).
- Subfiles:** Select the group of patterns to be searched, for example, inorganics, zeolites, minerals, etc. (d).
- Element # in Formula:** Choose the minimum/maximum number of elements considered in the formula (default values are min=1 and max=24).
- Density:** Enter a minimum/maximum density for the mineral being searched (default values are min=1 and max=80).

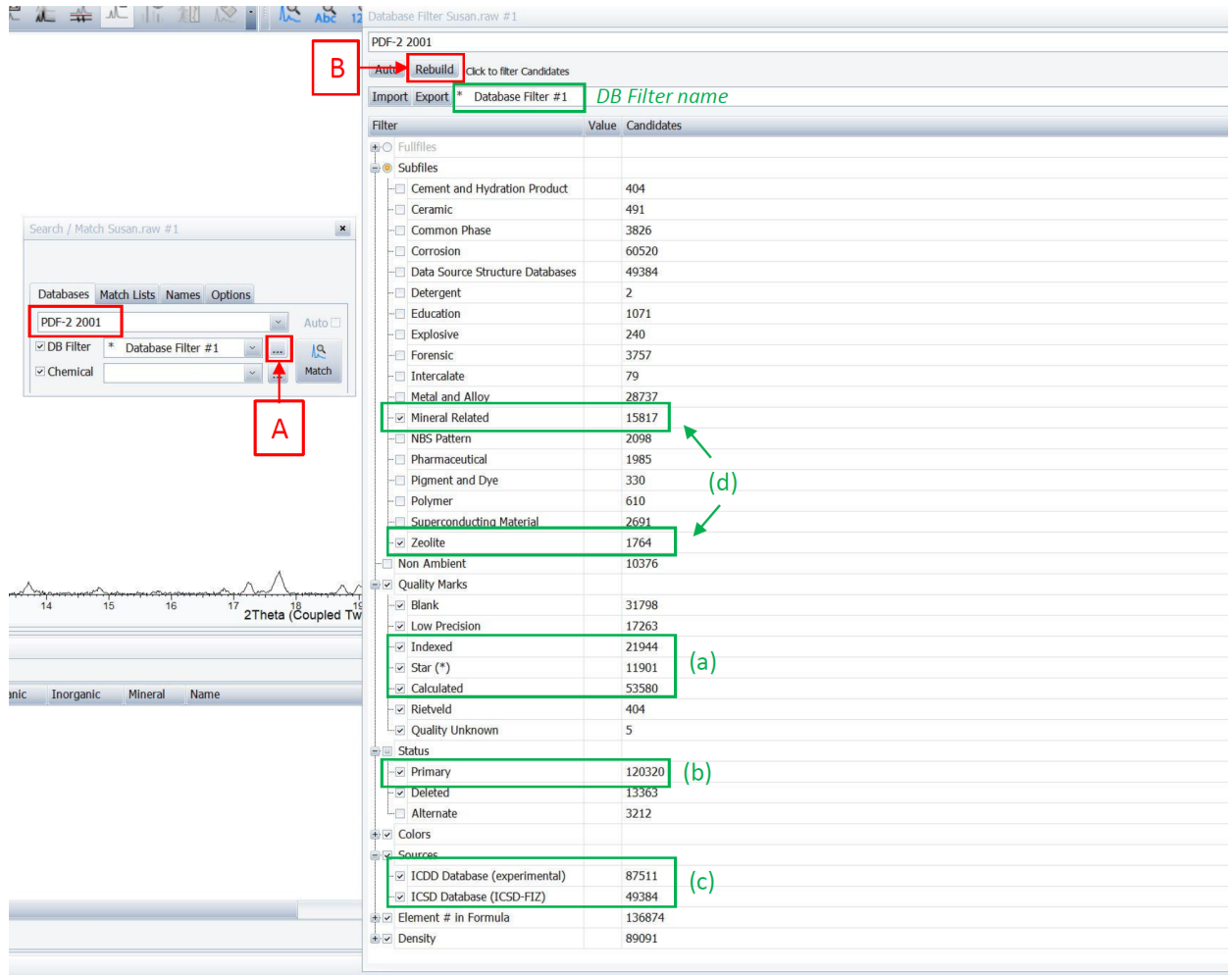


Figure 6. Database Filter.

Chemical Filter

In the **Databases** Tab, select **Chemical**. Click on the "three dots" button (Figure 7). The Chemical Filter window opens (Figure 7). The default name is 'Chemical Filter #1'. A chemical filter can be set for any element in the periodic table (Figure 7).

- Green = M = Mandatory.** All elements shall match.
- Red = D = Discarded.** Exclude from match.
- Blue = A = At least one element shall match** (must be present in the search result).
- Gray = N = Neutral.** Element may match.

To select an element, click on the element to change its status (e.g., M, D...) as desired.

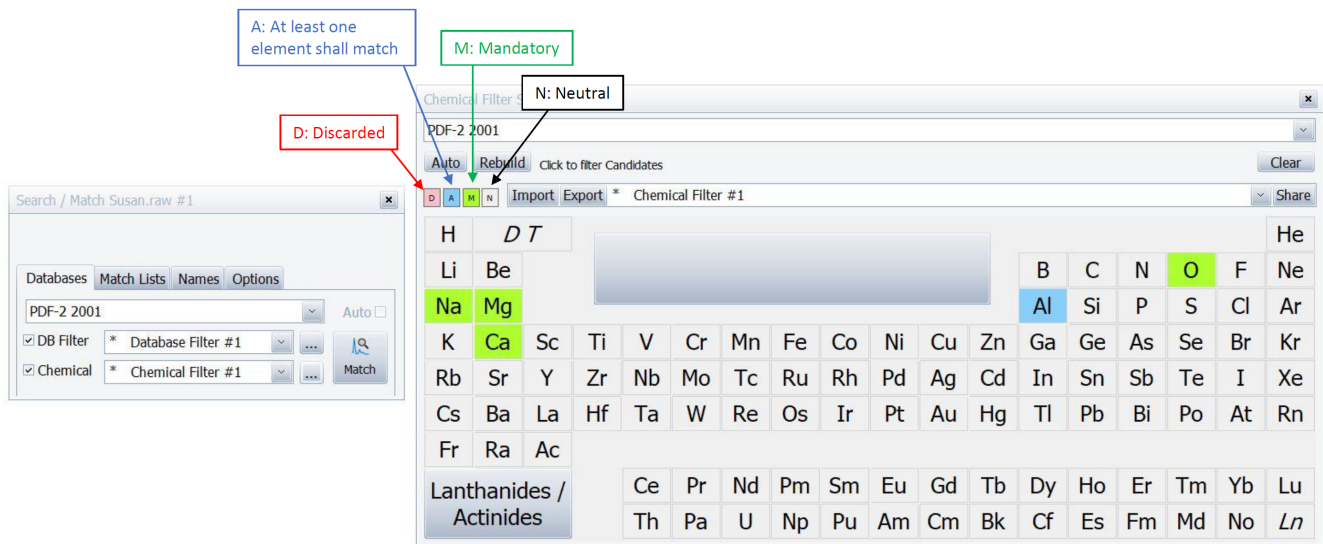


Figure 7. Chemical Filter.

Once the desired parameters are selected, click **Rebuild** to rebuild the database for your selections (Figure 6B). After the database is rebuilt, click back onto **Match Lists** (Figure 8). In the drop-down menu, select the list of clay minerals and common minerals and click OK (Figure 8A). Then, click **Match** (Figure 8B).

Close the window.

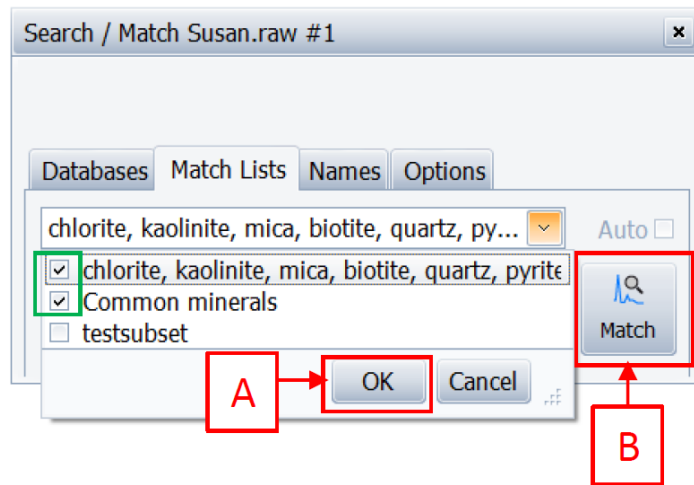


Figure 8. Match Lists

In the Auto Views panel, the list of candidates appears (Figure 9). Expand the table to see important information on the candidate (Figure 9), including:

- Index #**: Rank number of the given pattern during the Search run
- Match**: Number of reference pattern lines matching the unknown. The **Match** Column gives: on the left (green bar) the number of reference pattern lines matching the unknown in the displayed range, on the right (orange bar) the number of reference pattern lines not matching the unknown.
- FOM**: Figure of Merit – the higher this number, the better the match. Patterns are sorted by decreasing FOM. The FOM is represented by a blue bar proportional to its value.

Check the tick box (green square in Figure 8) to add selected peaks. To delete selected peaks, right-click on the selection and choose 'Delete'.

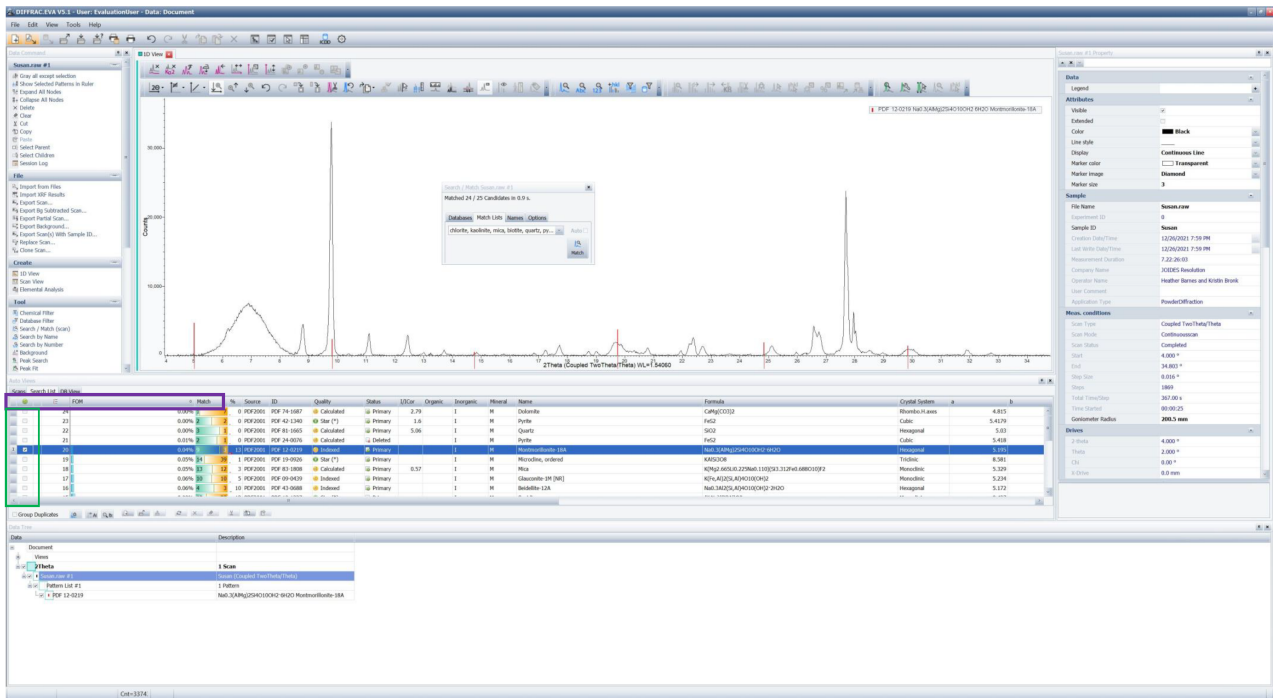




Figure 8. Search List Tab in the Auto Views Panel

Residual Scan – Searching the minor phases

Minor phases are sometimes difficult to identify because the patterns of the major peaks have a better position in the list. Using the **Residue** tool will exclude the already matched patterns and increase the weight of the minor phases.

Click  (Residual Scan) (Figure 9A) or right-click anywhere on the Graphical 1D View and then choose **Residual Scan > Residue (all scans)** (Figure

9B). Select the area you want to exclude. The area will be displayed in red. To restore the excluded part, click the Undo arrow  or right-click and choose **Residual Scan > Restore (all scans)**.

Check the tick box (green square in Figure 9) to add selected peaks. To delete selected peaks, right-click on the selection and choose 'Delete'.

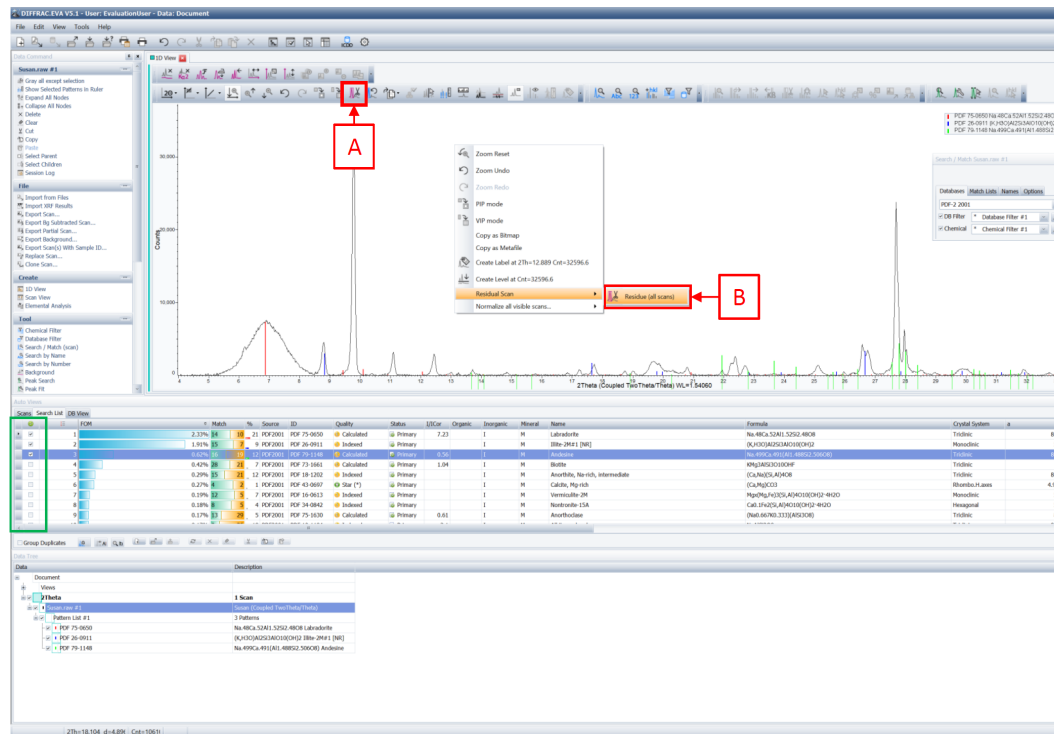


Figure 9. Residual Scan

Peak Search

Peak Search detects peaks automatically and is useful for phases not identified with Search/Match or to export the pattern to another program.

- Select the scan in the **Data Tree Panel**.
- Click **Peak Search** in the Tool List of the **Data Command Panel** (Figure 10A). The **Peak Search** dialog box is displayed.
- Move the slider to select the peaks you desire (Figure 10).
- Once you are satisfied, click **Make DIF** to create a DIF pattern (Figure 10B). The pattern list is created in the **Data Tree Panel** and can be Search/Matched.
- To select specific peaks click **Append to List** (Figure 10C) and a peak list is created in the **Data Tree Panel**.
- Select the DIF pattern in the **Data Tree Panel** (Figure 11A) and then click **Tool > Make Peaks** (Figure 11B).

The Peak Search with the Appended list appears in the Data Tree Panel (Figure 12).

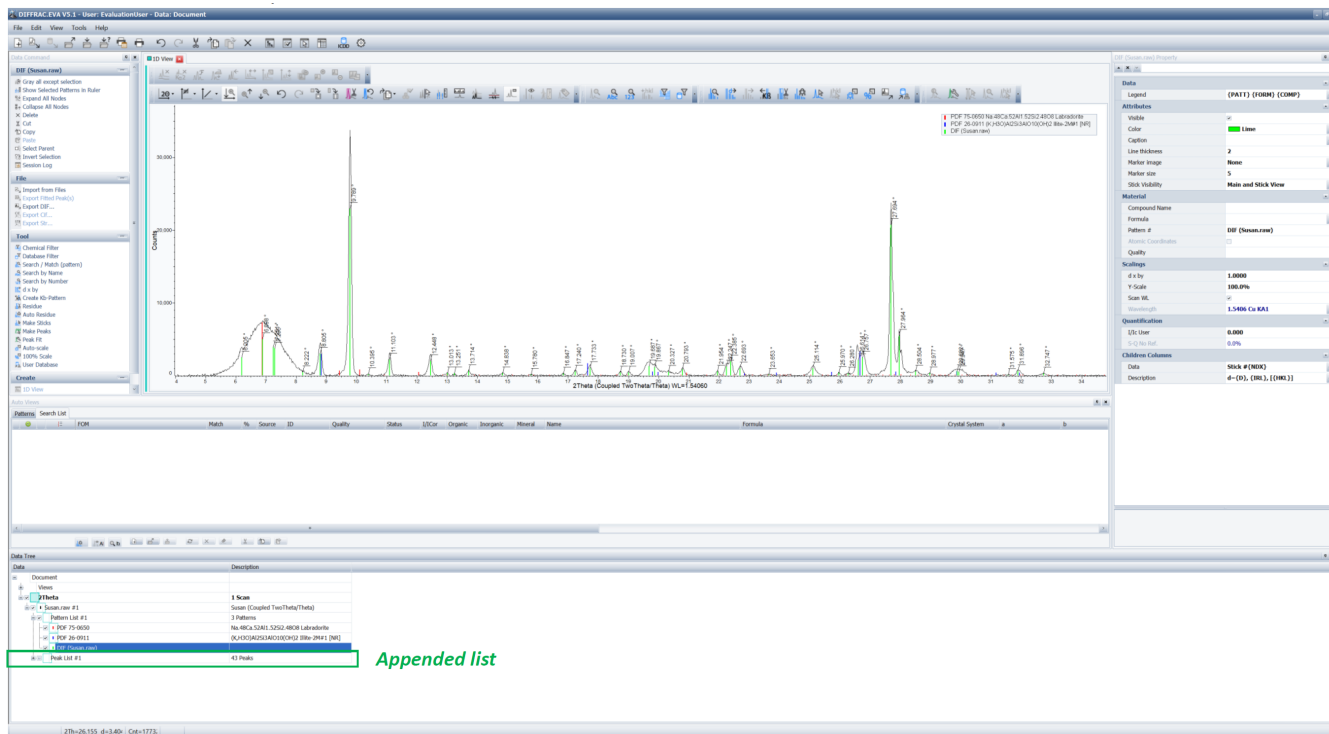




Figure 12. Peak Search with Append List.

Printing in EVA

You can print any of the views in EVA.

Click **Print Preview**  Button or click **File > Print Preview**. A 'Print Preview' window pops up. This allows you to enter header and footers onto your print out, in addition to editing axis and labels. You can then click on **Export as Image**  Button and save the print preview as an image .PNG file.

Credits

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