

# QualX Manual

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## QualX

**QualX** is a software for qualitative X-ray powder diffraction analysis. It allows phase identification of crystalline materials by comparing experimental diffraction patterns against reference databases.

## Features

- Import and visualize powder diffraction patterns
- Background estimation and subtraction
- Automatic and manual peak search
- Search/Match against crystallographic databases (COD, PDF-2)
- Figure of Merit (FOM) scoring for phase identification
- Quantitative phase analysis (RIR method)
- Project save/load (.qxp format)

## Quick Links

- Installation
- Database Installation
- Getting Started
- Search & Match

## Citing QualX

If you use QualX in your research, please cite one of the following works:

1. Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., Moliterni, A. and Rizzi, R., 'Main features of QUALX2.0 software for qualitative phase analysis' (2017). *Powder Diffr.* <https://doi.org/10.1017/S0885715617000240>
2. Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., Moliterni, A. and Rizzi, R., 'QUALX2.0: a qualitative phase analysis software using the freely available database POW\_COD' (2015). *J. Appl. Cryst.* **48**, 598-603. <https://doi.org/10.1107/S1600576715002319>
3. Altomare, A., Cuocci, C., Giacovazzo, C., Moliterni, A. and Rizzi, R., 'QUALX: A computer program for qualitative analysis using powder diffraction data' (2008). *J. Appl. Cryst.* **41**(4), 815-817. <https://doi.org/10.1107/S0021889808016956>

## Contact

IC-CNR Bari — <https://www.ic.cnr.it/>

| Name            | Email                                                                        |
|-----------------|------------------------------------------------------------------------------|
| Corrado Cuocci  | <a href="mailto:corrado.cuocci@cnr.it">corrado.cuocci@cnr.it</a>             |
| Angela Altomare | <a href="mailto:angela.altomare@cnr.it">angela.altomare@cnr.it</a>           |
| Anna Moliterni  | <a href="mailto:annagrazia.moliterni@cnr.it">annagrazia.moliterni@cnr.it</a> |

## Installation

### Windows

1. Download the Windows installer (`qualx-<version>_install.exe`) from the download page.

2. Run the installer and follow the on-screen instructions. The default installation folder is C:\Program Files\Qualx.
3. QualX will be available from the Start Menu and the desktop shortcut.

!!! note If a previous version of QualX is already installed, it must be uninstalled first before installing into the same folder.

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## macOS

1. Download the macOS DMG file (qualx-<version>\_macos.dmg) from the download page.
2. Double-click the DMG to mount it.
3. Drag the **QualX** icon into the **Applications** folder.
4. Eject the mounted volume.
5. Launch QualX from the Applications folder or Launchpad.

!!! note On first launch macOS may warn about an unidentified developer. Open **System Settings → Privacy & Security** and click **Open Anyway**.

---

## Linux

### Option A — AppImage (recommended)

The AppImage is a self-contained executable that bundles Qt6, the Fortran runtime and all other dependencies. It runs on most recent x86\_64 Linux distributions without installing anything.

#### 1. Download

Download qualx-<version>-x86\_64.AppImage (e.g. qualx-1.0.3-x86\_64.AppImage) from the download page.

#### 2. Make it executable and run it

```
chmod +x qualx-<version>-x86_64.AppImage
./qualx-<version>-x86_64.AppImage
```

!!! note AppImages require FUSE. If you get a “FUSE not found” error, either install libfuse2 (sudo apt-get install libfuse2 on Debian/Ubuntu) or extract and run the AppImage without FUSE: `bash ./qualx-<version>-x86_64.AppImage --appimage-extract ./squashfs-root/AppRun`

---

### Option B — Compilation from source (.tar.gz)

Use this method on any Linux distribution or when you need to choose a specific Fortran compiler.

## Requirements

| Tool               | Minimum version                           |
|--------------------|-------------------------------------------|
| CMake              | 3.20                                      |
| C++ compiler (g++) | 9                                         |
| Fortran compiler   | gfortran 9, ifort 2021, or ifx 2024       |
| Qt6                | 6.5 (Widgets, Sql, PrintSupport, Network) |

Install build dependencies on Debian/Ubuntu:

```
sudo apt-get install cmake build-essential gfortran pkg-config qt6-base-dev
```

On Fedora/RHEL:

```
sudo dnf install cmake gcc gcc-c++ make gcc-gfortran pkgconfig qt6-qtbase-devel
```

### Automated installation with `install.sh`

```
tar xzf qualx-<version>.tar.gz
cd qualx-<version>
./install.sh
```

The script configures, compiles, and installs QualX to `/opt/qualx-<version>`. To run it afterwards:

```
/opt/qualx-<version>/bin/qualx
# or add to PATH:
export PATH=/opt/qualx-<version>/bin:$PATH
```

By default `install.sh` uses `gfortran`. Pass a different compiler as the first argument, and an optional Qt6 prefix as the second:

```
./install.sh ifx # Intel Fortran (ifx)
./install.sh gfortran /home/user/Qt/6.5.0/gcc_64 # custom Qt path
```

### Manual CMake build

```
tar xzf qualx-<version>.tar.gz
cd qualx-<version>

cmake -DCMAKE_Fortran_COMPILER=gfortran \
      -DCMAKE_BUILD_TYPE=Release \
      -S . -B build
cmake --build build -j$(nproc)
sudo cmake --install build
```

---

## Databases

QualX requires at least one crystallographic reference database.

| Database                            | Format    | Notes                                              |
|-------------------------------------|-----------|----------------------------------------------------|
| COD (Crystallography Open Database) | COD/CIF   | Free — download separately, not bundled with QualX |
| PDF-2                               | PDF-2 DAT | Commercial — ICDD license required                 |

Database files are managed through **Search → Manage Databases**.

For instructions on installing a database, see Database Installation.

## First Launch

On first launch QualX will ask you to configure the path to the database files. See Getting Started for a step-by-step guide.

## Database Installation

QualX requires at least one crystallographic reference database in its own compiled format (.sq file). Database files are not included in the QualX installation and must be downloaded separately.

### Available databases

Pre-built databases are available for download from the QualX Databases page.

| File          | Contents                    | Size   |
|---------------|-----------------------------|--------|
| cod_inorg.zip | COD — inorganic phases only | 304 MB |
| cod.zip       | COD — complete database     | 2.7 GB |

Each archive contains a single folder (cod\_inorg or cod) with all the required files. Extract it into your QualXDB folder following the instructions below.

### Default database folder

QualX looks for databases in a dedicated folder called **QualXDB** inside your home directory:

| Platform      | Default path                |
|---------------|-----------------------------|
| Linux / macOS | ~/QualXDB                   |
| Windows       | C:\Users\<username>\QualXDB |

**At every launch** QualX scans this folder recursively for .sq files and registers any database it finds automatically — no manual configuration needed. You can organise the folder freely: subfolders are fully supported.

## Setting up the QualXDB folder

1. Create the QualXDB folder in your home directory.
2. Download one of the zip archives from the link above and extract it directly into QualXDB. After extraction the folder should look like:

```
~/QualXDB/  
├── cod_inorg/          (or cod/)  
│   ├── cod_inorg.sq  
│   ├── cod_inorg.sq.info  
│   ├── cod_inorg.sq.infostat  
│   └── cod_inorg.sq.search
```

3. Launch QualX — the database is detected and registered automatically.

## What happens if the folder is not found

If QualX starts without any configured database and the QualXDB folder does not exist, a dialog is shown with two options:

- **Choose folder...** — lets you select a different folder that will be saved as the new default. QualX scans it immediately and registers all databases found inside.
- **Manage Databases later** — dismiss the dialog and configure databases manually via **Search → Manage Databases**.

## Adding a database manually

If you prefer not to use the default folder, or need to register an additional database stored elsewhere:

1. Open **Search → Manage Databases**
2. Click **Add existing** and browse to your .sq database file
3. Click **OK** — the database is now active

## Introduction

QualX is designed around a simple workflow:

Import pattern → Data Reduction → Search & Match → Accept phases

## Main Window

The main window is divided into several panels:

- **Graphic area** (centre): displays the diffraction pattern, background, peaks and accepted phase reflections

- **Results List** (bottom/right dock): ranked list of candidate phases
- **Peaks** (dock): list of experimental peaks
- **Peak Compare** (dock): overlay of selected card reflections vs. experimental peaks
- **Quantitative** (dock): accepted phases with RIR percentages. The RIR value is actively used to perform a semi-quantitative analysis, shown as a pie chart
- **Report** (dock): summary report of the analysis

## Workflow Overview

1. **Import** a diffraction pattern (File → Import Diffraction Pattern)
2. **Background**: estimate and optionally subtract the background
3. **Peak Search**: detect peak positions and intensities
4. **Search/Match**: query the database and rank candidate phases by FOM
5. **Accept**: move identified phases to the Quantitative panel
6. **Save** the project (.qxp) to resume later

See the individual sections for detailed instructions.

## Getting Started

### Step 1 — Install a reference database

Before running the first search, at least one crystallographic reference database must be installed. QualX automatically detects databases placed in the **QualXDB** folder inside your home directory.

For download links, installation instructions and advanced configuration see the Database Installation page.

### Step 2 — Import a diffraction pattern

1. **File → Import Diffraction Pattern** (or drag-and-drop a file onto the graphic area)
2. Supported formats: .xy, .dat, .xrdml, .gda, .xye, .rtv
3. The pattern appears in the graphic area

### Step 3 — Background

1. **Pattern → Background → Generate Background**
2. Adjust parameters in the Background dialog
3. Optionally subtract: **Pattern → Subtract Background**

### Step 4 — Peak Search

1. **Pattern → Peaks → Peak Search**
2. The detected peaks appear as vertical markers in the graphic area
3. Fine-tune with **Pattern → Peaks → Peak Search Conditions**

## Step 5 — Search & Match

1. **Search** → **Search & Match**
2. QualX queries the database and shows ranked results in the **Results List**
3. Select a card to view its reflections overlaid on the experimental pattern

If Step 3 and/or Step 4 are skipped and **Search & Match** is run directly, QualX automatically performs the missing steps (Background and/or Peak Search) before running the search.

## Step 6 — Accept a phase

1. Select a card in the Results List
2. Click **Accept** (☑ button) — the phase moves to the **Quantitative** panel
3. If residual search is enabled in the **Search & Match Options** dialog, QualX automatically performs a residual search on remaining peaks — see the Search & Match page for details

## Step 7 — Save the project

**File** → **Save Project As** saves a .qxp file containing the pattern data, peaks, results and accepted phases.

## Examples

QualX installs three test diffraction patterns together with the application, in the share/qualx/examples folder inside the installation directory (for example <install\_dir>/share/qualx/examples on Linux). They can be opened directly with **File** → **Import Diffraction Pattern**.

All three patterns are laboratory data collected with CuK $\alpha$  radiation, and all are multi-phase mixtures with known (“true”) weight fractions — they are useful both for trying out the Search & Match workflow described in Getting Started and for checking the accuracy of the Quantitative Phase Analysis (RIR) results against a reference composition.

### Example 1 — example1.dat

A three-phase mixture prepared in the laboratory.

| Phase                | True weight fraction |
|----------------------|----------------------|
| Corundum             | 50.0%                |
| Silicon              | 30.0%                |
| Lanthanum hexaboride | 20.0%                |

This is the simplest of the three mixtures and a good first test of the default Search & Match settings (no restraints needed).

### Example 2 — CPD2.dat

A four-phase sample from a round-robin study on Quantitative Phase Analysis (QPA) organized by the IUCr Commission on Powder Diffraction. The diffraction data are affected by preferred orientation effects, which makes the quantitative step less straightforward than Example 1.

| Phase    | True weight fraction |
|----------|----------------------|
| Corundum | 21.27%               |
| Zincite  | 19.94%               |
| Fluorite | 22.53%               |
| Brucite  | 36.26%               |

### Example 3 — MIXT\_5.dat

A five-phase mixture prepared in the laboratory — the most demanding of the three examples, useful for testing Search & Match restraints (e.g. chemical composition or cell parameters) when the unrestrained result list becomes too large to inspect by hand.

| Phase                | True weight fraction |
|----------------------|----------------------|
| Corundum             | 28.40%               |
| Lanthanum hexaboride | 18.70%               |
| Zincite              | 13.10%               |
| Calcite              | 30.90%               |
| Silicon              | 8.90%                |

### Suggested workflow

1. Import one of the example patterns (**File → Import Diffraction Pattern**).
2. Run background subtraction and peak search as described in Getting Started.
3. Run **Search → Search & Match** against a reference database containing the expected phases (e.g. corundum, silicon, zincite, fluorite, brucite, calcite, lanthanum hexaboride).
4. Accept the matching phases one by one and compare the RIR weight fractions shown in the **Quantitative** panel against the true values listed above.

### Data Reduction

Before running a Search & Match, the raw diffraction pattern usually needs to be processed. QualX provides the following data reduction tools:

| Tool                    | Menu                              | Description                           |
|-------------------------|-----------------------------------|---------------------------------------|
| Background              | Pattern → Background              | Estimate and subtract background      |
| Peak Search             | Pattern → Peaks                   | Detect peak positions and intensities |
| Smoothing               | Pattern → Smoothing               | Reduce noise                          |
| K- $\alpha$ 2 Stripping | Pattern → K- $\alpha$ 2 Stripping | Remove the K $\alpha$ 2 contribution  |

All tools are accessible from the **Pattern** menu.

## Background

### Overview

Background estimation is performed by fitting a polynomial (Chebyshev) or filter-based curve to the diffraction pattern. The estimated background can be visualised and subtracted before peak search.

### Controls

Open **Pattern → Background → Generate Background** to display the Background dialog.

| Parameter           | Description                                      |
|---------------------|--------------------------------------------------|
| <b>Type</b>         | Background model: Chebyshev polynomial or filter |
| <b>Coefficients</b> | Number of polynomial terms (Chebyshev mode)      |
| <b>Range</b>        | 2 $\theta$ range to use for background fitting   |

It is possible to choose the background function that best fits the selected background points. The default function is the Chebyshev polynomial. The other available background functions are: polynomial, cosine Fourier series, cubic spline, Bézier spline, and a filter function based on the Brückner algorithm (Brückner, 2000).

### Manual editing

Background points selected automatically can be added or deleted using the mouse.

### Subtraction

Click **Pattern → Subtract Background** (or press the button in the toolbar) to subtract the estimated background from the pattern. The original pattern is preserved and can be restored by reloading the project.

!!! note Background subtraction is recommended before running Peak Search, as it improves peak detection accuracy.

# Peak Search

## Overview

QualX locates peaks in the diffraction pattern and records their  $2\theta$  position, intensity and FWHM. These peaks are used as input for the Search & Match.

## Running Peak Search

**Pattern → Peaks → Peak Search** runs the automatic peak search with the current conditions. Detected peaks appear as vertical markers in the graphic area and are listed in the **Peaks** dock.

## Peak Search Conditions

**Pattern → Peaks → Peak Search Conditions** opens the conditions dialog.

| Parameter                                                    | Description                                                |
|--------------------------------------------------------------|------------------------------------------------------------|
| <b>Min. <math>2\theta</math> / Max. <math>2\theta</math></b> | Search range                                               |
| <b>Threshold</b>                                             | Minimum peak height relative to the pattern maximum        |
| <b>Sensitivity</b>                                           | Controls smoothing before peak detection                   |
| <b>Max. peaks</b>                                            | Maximum number of peaks to detect                          |
| <b>Append</b>                                                | Add new peaks to the existing list instead of replacing it |

## Manual editing

- **Add peak:** View → Selection Mode, then right-click on the pattern
- **Delete peak:** select a peak marker and press Delete
- **Load / Save:** Pattern → Peaks → Load Peaks / Save Peaks

!!! tip If too many or too few peaks are found, adjust **Threshold** and **Sensitivity** in the Peak Search Conditions dialog.

## Smoothing

### Overview

Smoothing of the experimental pattern by the Savitzky-Golay filter method (Savitzky and Golay, 1964), or by the adjacent-averaging method.

## Search & Match

QualX identifies crystalline phases by comparing the experimental peak list against a reference database and ranking candidates by a **Figure of Merit (FOM)**.

## Menu

| Action                                     | Description                                                  |
|--------------------------------------------|--------------------------------------------------------------|
| <b>Search → Search &amp; Match</b>         | Run a full search using current peaks and options            |
| <b>Search → Search &amp; Match Options</b> | Configure FOM weights, $\Delta 2\theta$ , min. FOM           |
| <b>Search → Restraints</b>                 | Restrict the search to specific elements, space groups, etc. |
| <b>Search → Manage Databases</b>           | Add, remove or switch reference databases                    |

## Results List

After a search, the **Results List** dock shows ranked candidates with columns:

| Column           | Description                                      |
|------------------|--------------------------------------------------|
| (colour)         | Unique colour assigned to the card               |
| QM               | Quality mark of the reference card               |
| ID               | Card identifier                                  |
| Chemical Name    | Compound name                                    |
| Chemical Formula | Chemical formula                                 |
| Peakpos.         | Peak-position component of FOM                   |
| Intensity        | Intensity component of FOM                       |
| Scale            | Intensity scale factor                           |
| FOM              | Total Figure of Merit (higher = better match)    |
| S-Quant.         | Semi-quantitative percentage (RIR, if available) |

See Search Match and Restraints for details.

## Search & Match

### How it works

QualX performs a multi-step search:

1. **Strongest peaks filter:** for each database card, only the  $N$  strongest reference peaks are compared against the experimental peak list (fast pre-filter).
2. **FOM calculation:** a weighted Figure of Merit combines peak-position matching and intensity matching.
3. **Ranking:** cards are sorted by descending FOM; only cards above **Min. FOM** are shown.

### Figure of Merit

At the end of the search-match step a list of plausible database crystalline phases are ranked according to the decreasing values of a FoM. The FoM includes four contributions, three of them suitably weighted, according to the following formula:

$$\text{FoM} = \sqrt{\frac{\text{FoM}_{db} \cdot (w_{\theta} \text{FoM}_{\theta} + w_I \text{FoM}_I + w_{ph} \text{FoM}_{ph})}{w_{\theta} + w_I + w_{ph}}}$$

where FoM $_{\theta}$  takes into account the average difference between the 2 $\theta$  values of the observed and matched database peaks; FoM $_I$  is related to the average difference between the intensity values of the observed and matched database peaks; FoM $_{ph}$  depends on the percentage of the matched experimental peaks and on their intensity; and FoM $_{db}$  depends on the percentage of the matched database peaks and on their intensity.

FoM $_{\theta}$  is the contribution coming from the 2 $\theta$  differences between the experimental and the associated database peaks:

$$\text{FoM}_{\theta} = 1 - \frac{\sum_i^{N_{db}^{ass}} |2\theta_i^{\text{exp}} - 2\theta_i^{db}|}{N_{db}^{ass} \cdot \Delta}$$

where the summation is over the associated database peaks (a database peak is considered associated if its 2 $\theta$  distance from the experimental peak is less than  $\Delta$ ), 2 $\theta^{\text{exp}}$  and 2 $\theta^{db}$  are the positions of the experimental and database peaks, respectively.

FoM $_I$  is the contribution due to the differences between the intensities of the experimental and the associated database peaks:

$$\text{FoM}_I = 1 - \frac{\sum_i^{N_{\text{exp}}^{ass}} |I_i^{\text{exp}} - I_i^{db}|}{N_{\text{exp}}^{ass}}$$

where  $I_{\text{exp}}$  and  $I_{db}$  are the experimental and database intensity respectively, the summation is over the associated experimental peaks.

FoM $_{ph}$  is the contribution due to the intensities of the associated experimental peaks and their percentage:

$$\text{FoM}_{ph} = \sqrt{\frac{\sum_{i=1}^{N_{\text{exp}}^{ass}} I_i^{\text{exp}}}{N_{\text{exp}}} \cdot \frac{N_{\text{exp}}^{ass}}{N_{\text{exp}}}}$$

where  $N_{\text{exp}}$  is the total number of experimental peaks.

FoM<sub>db</sub> is the contribution due to the intensities of the associated database peaks and their percentage:

$$\text{FoM}_{db} = \sqrt{\frac{\sum_{i=1}^{N_{db}^{ass}} I_i^{db}}{N_{db}} \cdot \frac{N_{db}^{ass}}{N_{db}}}$$

where I<sub>db</sub> is the database intensity and the summation at the numerator is over the associated database peaks; N<sub>db</sub> is the total number of the database peaks.

The weighting factors w<sub>θ</sub>, w<sub>I</sub>, w<sub>ph</sub> and Δ (default heuristic values are set for them) can be adjusted directly by the user via the graphical interface. w<sub>ph</sub> is related to the number of expected phases.

The default value of the weights w<sub>θ</sub>, w<sub>I</sub>, and w<sub>ph</sub> is 0.5, but it can be changed by the dialogue window in Figure 1 (via the “2θ”, “Intensity” and “Phases” trackbars).

## Search Options

Open **Search** → **Search & Match Options**:

| Option                       | Description                                                             |
|------------------------------|-------------------------------------------------------------------------|
| <b>Min. FOM</b>              | Discard cards below this threshold                                      |
| <b>2θ / d weight</b>         | Contribution of peak-position agreement to FOM                          |
| <b>Intensity weight</b>      | Contribution of intensity agreement to FOM                              |
| <b>Phases weight</b>         | Bias towards single-phase vs. multi-phase solutions                     |
| <b>Δ2θ</b>                   | Peak matching tolerance in degrees (Auto = calculated from peak widths) |
| <b>Max. entries</b>          | Maximum number of results to display                                    |
| <b>Check strongest peaks</b> | Use only the N strongest peaks for the pre-filter                       |
| <b>Check deleted cards</b>   | Include cards marked as deleted in the database                         |
| <b>Residual searching</b>    | After accepting a phase, automatically re-search on residual peaks      |

## Accepting a Phase

1. Select a card in the Results List.
2. Click **Accept** (☑). The card is moved to the **Quantitative** dock.
3. If **Residual searching** is enabled, QualX subtracts the accepted phase contribution and repeats the search on the remaining peaks.

## Restraints

Restraints narrow the database search by pre-filtering cards that do not match specified chemical or crystallographic criteria.

Open **Search** → **Restraints**.

### Properties tab

| Field                  | Description                                  |
|------------------------|----------------------------------------------|
| <b>Chemical name</b>   | Filter by compound name (partial match)      |
| <b>Color</b>           | Filter by crystal color                      |
| <b>Density (calc.)</b> | Filter by calculated density $\pm$ tolerance |
| <b>Density (meas.)</b> | Filter by measured density $\pm$ tolerance   |

### Composition tab

| Field           | Description                                                        |
|-----------------|--------------------------------------------------------------------|
| <b>Elements</b> | Include/exclude chemical elements                                  |
| <b>Mode</b>     | Contains (AND/OR), Only (exact composition), Just (at least these) |

### Symmetry tab

| Field                  | Description                                                                        |
|------------------------|------------------------------------------------------------------------------------|
| <b>Crystal system</b>  | Filter by crystal system (cubic, tetragonal, ...)                                  |
| <b>Space group</b>     | Filter by space group symbol                                                       |
| <b>Cell parameters</b> | Filter by unit cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma \pm$ tolerance |

### Entries tab

Paste a list of card IDs (one per line) to restrict the search to those specific entries.

### Subfiles tab

Filter by PDF-2 subfile codes (e.g., I = inorganic, O = organic).

### Buttons

| Button            | Action                                                            |
|-------------------|-------------------------------------------------------------------|
| <b>Load cards</b> | Query the database with the current restraints (replaces results) |

| Button                    | Action                                               |
|---------------------------|------------------------------------------------------|
| <b>Load &amp; Merge</b>   | Query and add results to the current list            |
| <b>Search &amp; Match</b> | Run a FOM-ranked search within the restrained subset |

## References

### QualX

1. Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., Moliterni, A. and Rizzi, R., ‘Main features of QUALX2.0 software for qualitative phase analysis’ (2017). *Powder Diffr.* <https://doi.org/10.1017/S0885715617000240>
2. Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., Moliterni, A. and Rizzi, R., ‘QUALX2.0: a qualitative phase analysis software using the freely available database POW\_COD’ (2015). *J. Appl. Cryst.* **48**, 598-603. <https://doi.org/10.1107/S1600576715002319>
3. Altomare, A., Cuocci, C., Giacovazzo, C., Moliterni, A. and Rizzi, R., ‘QUALX: A computer program for qualitative analysis using powder diffraction data’ (2008). *J. Appl. Cryst.* **41**(4), 815-817. <https://doi.org/10.1107/S0021889808016956>

### Databases

- **COD** — Crystallography Open Database: <https://www.crystallography.net/cod/>
- **PDF-2** — ICDD Powder Diffraction File: <https://www.icdd.com/>

### Software libraries

- **Qt** — <https://www.qt.io/>
- **QCustomPlot** — <https://www.qcustomplot.com/>