Qualx2

a qualitative phase analysis software

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Introduction

http://www.ba.ic.cnr.it/softwareic/qualx/introduction/

QualX (Altomare *et al., 2015*) is a program for qualitative phase analysis by powder diffraction data. QualX is able to carry out the phase identification by inquiring the PDF-2 commercial database and a new freely available database: POW_COD. POW_COD has been developed by the authors of QualX program and created by using the structure information contained in the Crystallography Open Database (COD) (Grazulis *et al.*, 2009, 2012). The PDF database is maintained and continuously updated by the International Center for Diffraction Data (ICDD) (ICDD, 2003). The main novelty of QualX, with respect to its previously distributed version (Altomare *et al.*, 2008), is the possibility of managing the POW_COD database.

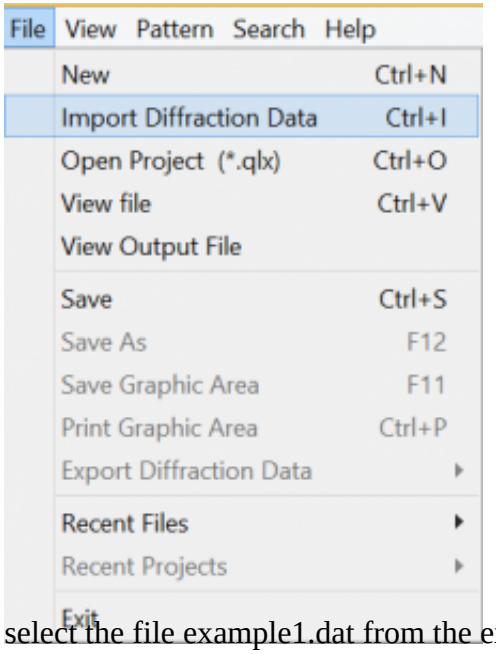
For problems or suggestions please contact corrado.cuocci@ic.cnr.it, nicola.corriero@ic.cnr.it.

If you use this program, please cite
Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., Moliterni, A., Rizzi, R.
QUALX2.0: a qualitative phase analysis software using the freely available database POW_COD, J. Appl. Cryst. (2015). **48**, 598-603.

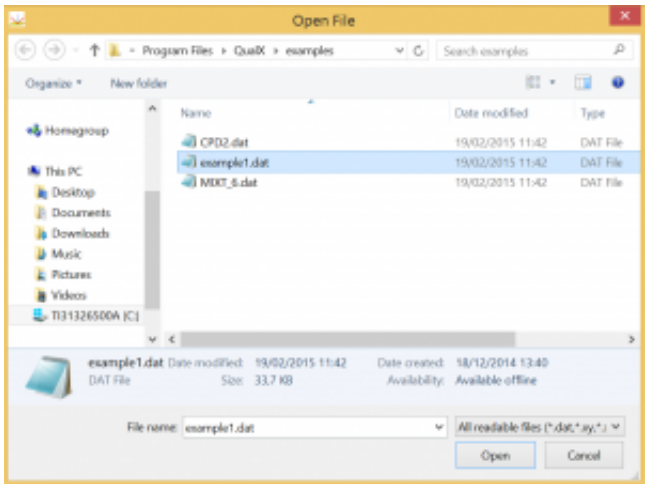
Starting soon with QualX

http://www.ba.ic.cnr.it/softwareic/qualx/introduction/starting-soon-with-qualx/

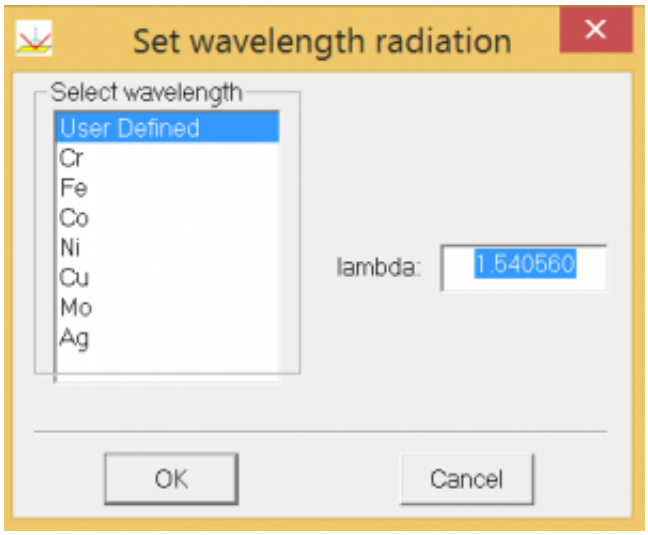
1) Run the program by clicking on QualX icon 
2) Press ‘File’ > ‘Import diffraction data’



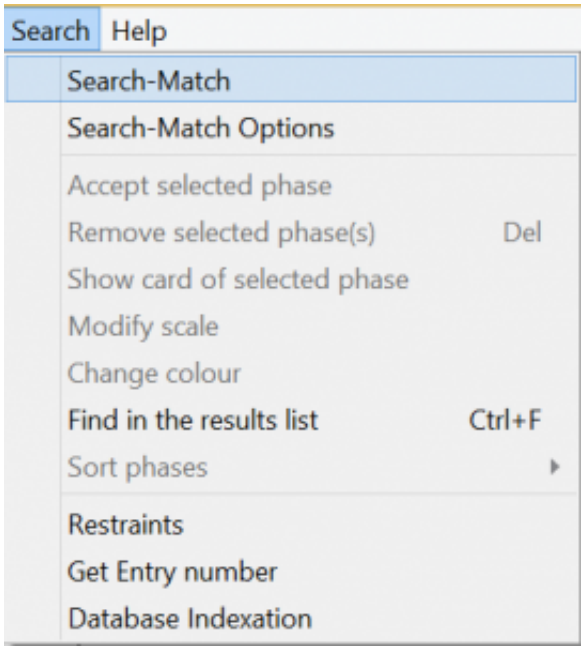
select the file example1.dat from the examples folder.



and select wavelength



3) Press ‘Search’>’Search-Match’



If the database is not installed an error message window will appear (see the instructions for the database installation). After the installation the step Search-Match must be repeated.
The program carries out automatically the following steps: 1) estimation of the background and subtraction of the background contribution from the experimental pattern; 2) location of the experimental diffraction peaks (peak search) supplying the (d,I) set; 3) search for the candidate database single phase pattern(s) best matching the experimental powder data (search).
At the end of the Search-Match step, the results list of feasible phases sorted according to a figure of merit (FoM) is shown. The FoM assesses the goodness of the identified phase(s) by taking into account the number of matched peaks, the average difference in 2q peak position and the average difference in peak intensity between the observed and database peaks.

No.	QM	CARD	Compound Name	Chemical Formula	Peakpos.	Intensity	Scale	FoM	S-Quant.
1	C	00-100-0055		B6 La	0.90909	0.71347	0.80424	0.81338	10.522
2	C	00-110-1023	Lanthanum boride (1/6)	La B6	0.93205	0.67985	0.80066	0.81120	10.190
3	C	00-410-4917		Si	0.97169	0.82206	1.0282	0.79314	4.738
4	C	00-900-7496	[Corundum]	Al2 O3	0.80364	0.77142	0.37574	0.78724	1.097
5	C	00-210-4748	Silicon [Silicon]	Si	0.97116	0.78868	1.0402	0.78642	4.669
6	C	00-230-0375		Al2 O3	0.80539	0.76873	0.37623	0.77816	1.089
7	C	00-100-8993	Europium boride carbide (1/5.8/0.2)	Eu B5.8 C0.2	0.77276	0.67818	0.79612	0.77742	12.564
8	C	00-100-8907	Europium boride carbide (1/5.8/0.2)	Eu (B5.8 C0.2)	0.77276	0.67818	0.79612	0.77742	12.564
9	C	00-230-0448	aluminium oxide loop [corundum]	Al2 O3	0.78601	0.77649	0.37394	0.76913	1.093
10	C	00-900-8094	[Corundum]	Al1.82 Cr0.18 O3	0.76183	0.65537	0.41732	0.74700	1.195
11	C	00-100-8114	Sodium thorium boride (.77/.23/6)	Na.77 Th.23 B6	0.53117	0.61833	0.87626	0.71076	4.689
12	C	00-151-1297	Pd3 Sm B	B Pd3 Sm	0.87479	0.27805	0.43640	0.71065	18.389
13	C	00-101-1233	Zinc iron sulfide (.7/.3/1) [Sphalerite (F]	Zn0.66 Fe0.34 S	0.96705	0.76491	1.0560	0.70155	9.177
14	C	00-210-4216	cerium hexaboride	B6 3-, Ce 3+	0.42453	0.68580	0.80268	0.70151	10.677
15	C	00-150-9034	Silver cadmium indium (0.75/0.1/0.15)	Ag0.75 Cd0.1 In0.15	0.78032	0.68823	0.41698	0.69161	18.659

Use the search menu (toolbar on the right-hand side) to manage the list.
4) Press the button each time you want to accept a phase from the results list. If the corresponding entry contains the I/Ic value, the semi-quantitative analysis is performed by the program and the percentage is given in the last column. In case of POW_COD the I/Ic value is available for each entry.

No.	QM	CARD	Compound Name	Chemical Formula	Peakpos.	Intensity	Scale	FoM	S-Quant.
P.1	C	00-100-0055		B6 La	0.90909	0.71347	0.80424	0.81338	12.7%
P.2	C	00-410-4917		Si	0.97169	0.82206	1.0282	0.81756	36.1%
P.3	C	00-900-7496	[Corundum]	Al2 O3	0.80364	0.73179	0.33744	0.82855	51.2%

Examples

http://www.ba.ic.cnr.it/softwareic/qualx/introduction/examples/

The following test mixtures are provided in Install_dir\QualX\examples\ where

Install_dir is the default installation folder on your operating system (e.g., C:\Program Files\)

1. *example1.dat* (laboratory data, CuKa1 radiation). It is an example of a laboratory-prepared three-phase mixture. Its composition is: corundum, silicon and lanthanum hexaboride; the corresponding true weight fractions are 50.0%, 30.0%, 20.0%.
2. *CPD2.dat* (laboratory data, CuKa radiation). It is a four-phase mixture belonging to a set of test samples prepared for a round robin on Quantitative Phase Analysis (QPA) organized by the International Union of Crystallography (IUCr) Commission on Powder Diffraction (CPD) (Madsen
   et al., 2001; Scarlett et al., 2002). X-ray diffraction data are affected by preferred orientation effects. The mixture composition is: corundum, zincite, fluorite and brucite; the corresponding true weight fractions are 21.27%, 19.94%, 22.53% and 36.26%.
3. ?*MIXT_5.dat* (laboratory data,CuKa1 radiation). It is an example of a laboratory-prepared five-phase mixture. Its composition is : corundum, lanthanum hexaboride, zincite, calcite and silicon. The corresponding true weight fractions are: 28.40%, 18.70%, 13.10%, 30.90% and 8.90%.?

Data Reduction

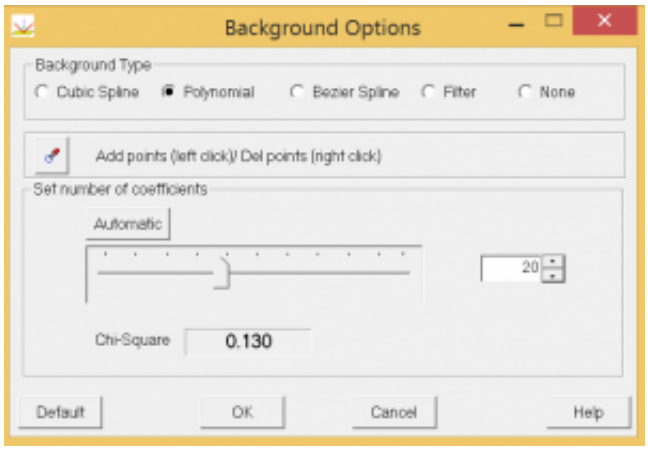
http://www.ba.ic.cnr.it/softwareic/qualx/data-reduction/

Background

http://www.ba.ic.cnr.it/softwareic/qualx/data-reduction/background/

Press ‘Pattern’ > ‘Create Background’ to estimate automatically the background. Then select ‘Pattern’>’Subtracted Background’ to subtract the background contribution from the experimental pattern. The background can be modified manually selecting ‘Pattern’>’Background Options’.

Background Options Dialogue



Background Type: four different types of background are available.

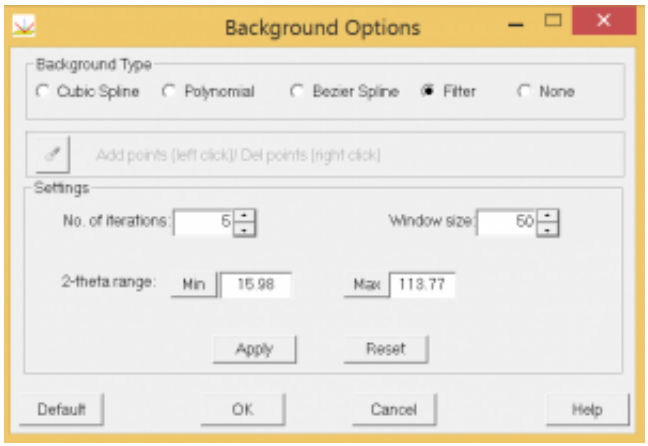
Cubic Spline:	the selected background points are used for a cubic spline interpolation.
Polynomial:	the selected background points are fitted via Chebyshev polynomial function (default choice).
Bezier Spline:	the selected background points are interpolated via Bézier curve.
Filter:	activates a low-pass filter according to Brückner algorithm (Brückner, 2000).

If ‘None’ option is selected the background will be not estimated.

Add points/Del points: press button  to add or delete points from the graphic area for background calculation. Use right click mouse to delete points and left click mouse to add points. This option is not activated in case of background filter type.

Set number of coefficients: selects the number of coefficients for polynomial background. Press button AUTOMATIC for automatic selection of the polynomial degree. Chi-Square estimates the agreement between the calculated and experimental background points.

If ‘Filter’ type is selected the following window is shown by the program.

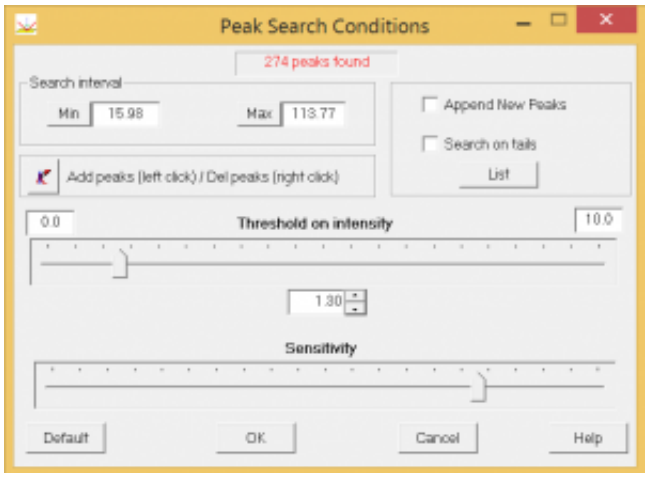


No. of iterations: number of iterations of filter background.
Window size: number of points used to smooth the background.
2-theta range: sets the range in which the background filter will be applied. Use Min button MIN and Max button MAX to select the 2? minimum and maximum, respectively.
Apply: press button APPLY to apply filter settings in the selected 2? range.
Reset: press button RESET to restore the default filter settings.
Default: restores the default Background Options.

Peak Search

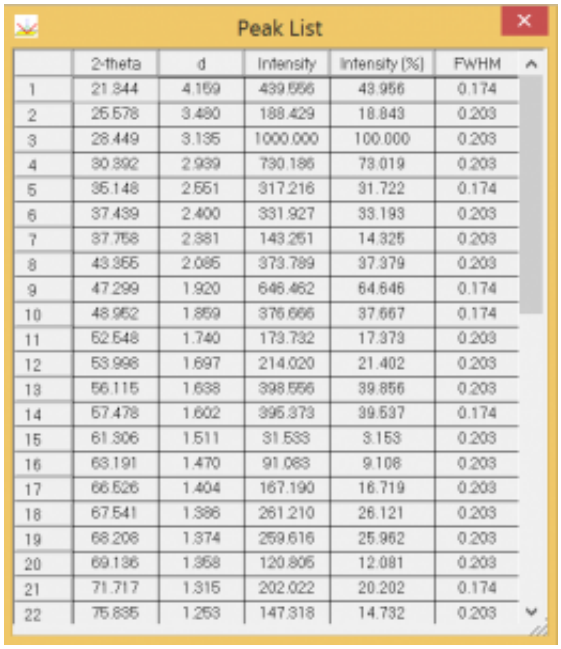
http://www.ba.ic.cnr.it/softwareic/qualx/data-reduction/peak-search/

Select ‘Pattern’>’Peak Search’ to activate the search of peaks on the pattern. To modify the default peak search approach press ‘Pattern’>’Peak Search Options’; the following window will appear.
Peak Search Options Dialogue:



Search interval: selects the interval where the peaks must be found. Press Min button and Max button to select the 2? minimum and maximum, respectively.

List: shows the list of found peaks. The calculated full width at half maximum (FWHM) is also given.


Peak List

	2-theta	d	Intensity	Intensity (%)	FWHM
1	21.344	4.159	439.556	43.956	0.174
2	25.578	3.480	188.429	18.843	0.203
3	28.449	3.135	1000.000	100.000	0.203
4	30.392	2.939	730.186	73.019	0.203
5	35.148	2.551	317.216	31.722	0.174
6	37.439	2.400	331.927	33.193	0.203
7	37.758	2.381	143.251	14.325	0.203
8	43.355	2.085	373.789	37.379	0.203
9	47.299	1.920	646.462	64.646	0.174
10	48.952	1.859	376.666	37.667	0.174
11	52.548	1.740	173.732	17.373	0.203
12	53.998	1.697	214.020	21.402	0.203
13	56.115	1.638	398.556	39.856	0.203
14	57.478	1.602	395.373	39.537	0.174
15	61.306	1.511	31.533	3.153	0.203
16	63.191	1.470	91.083	9.108	0.203
17	66.526	1.404	167.190	16.719	0.203
18	67.541	1.386	261.210	26.121	0.203
19	68.208	1.374	259.616	25.962	0.203
20	69.136	1.358	120.806	12.081	0.203
21	71.717	1.315	202.022	20.202	0.174
22	75.835	1.253	147.318	14.732	0.203

Append New Peaks: the new peaks found in the user supplied search interval are added to the already located peaks lying outside the search interval. If this option is not active the peaks previously located outside the search interval will be excluded.

Search on tails: uses second derivative algorithm to find hidden peaks on tails.

Add peaks/Del peaks: press button to add or delete peaks from the graphic area. Use left click mouse to add peaks and rigth click mouse to delete peaks.

Threshold on intensity: use the trackbar to modify the density of peaks. The numeric fields, are editable to modify the minimum and maximum intensity threshold.

Sensitivity: use the trackbar to modify the peak search sensitivity. This option is useful in presence of noisy pattern.

Help: button connected to this page.

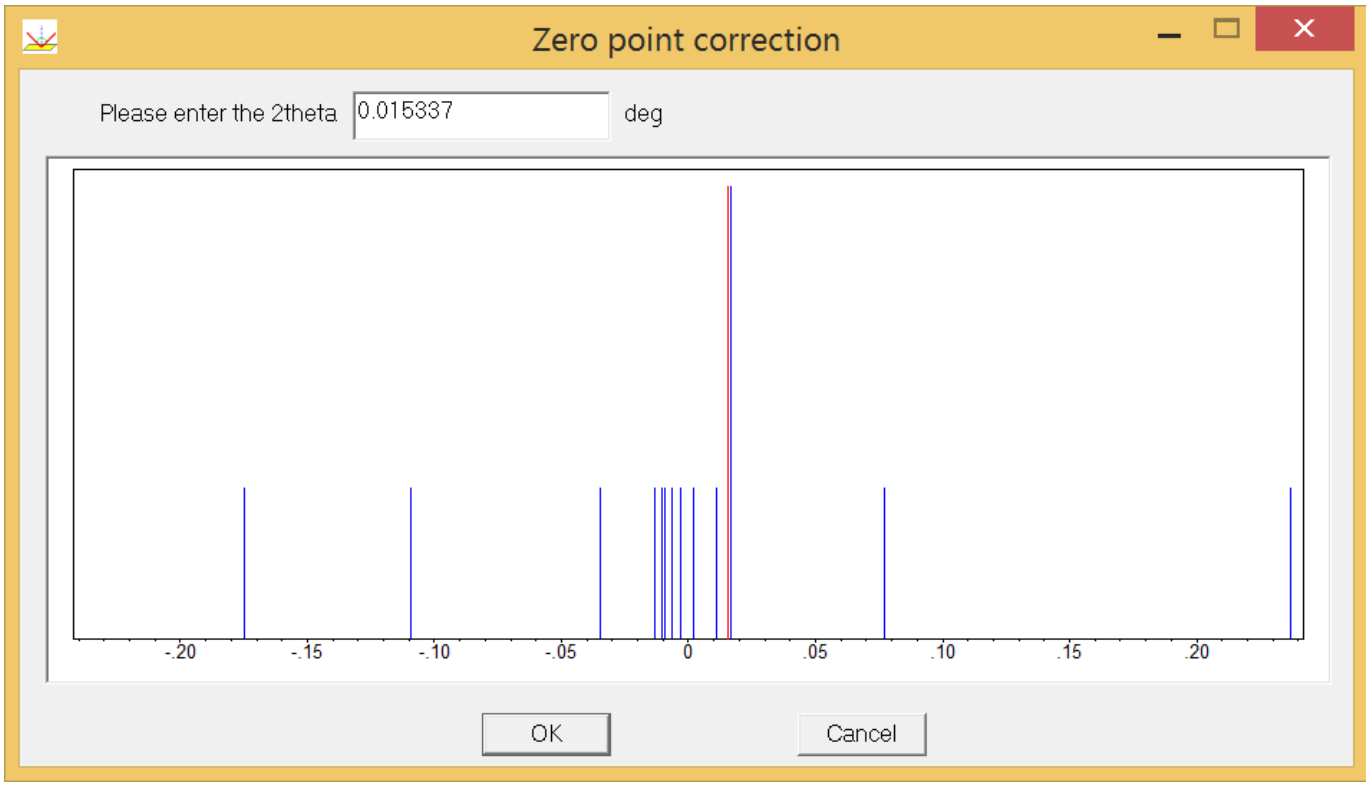
Default: restores the default settings.
Selecting ‘Pattern’>’Import peaks from file’ it is possible to load an ASCII file containing a peaks list (d values or 2? values).

2? Zero Correction

http://www.ba.ic.cnr.it/softwareic/qualx/data-reduction/2%ce%b8-zero-correction/

The selection ‘Pattern’>’Zero Point Correction’ gives the correction of zero shift. This option is enabled only after the peak search step. The eflection-pair method (Dong et. al., 1999) is applied.

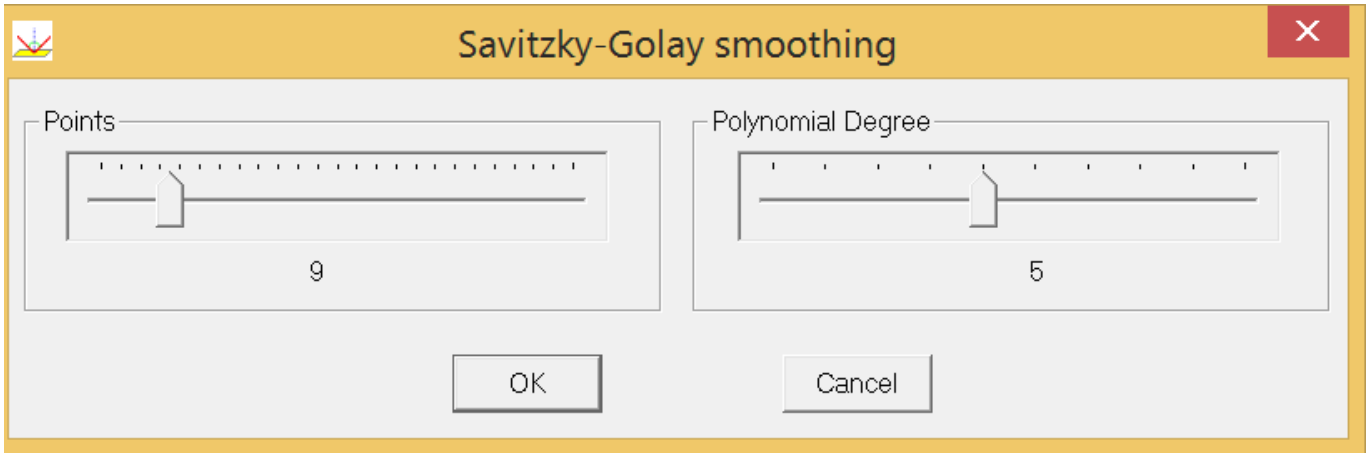
The suggested value corresponds to the point of maximum density of bars in the histogram. This value can be modified writing the new value in the entry box and clicking on ‘OK’ button.



Smoothing

http://www.ba.ic.cnr.it/softwareic/qualx/data-reduction/smoothing/

Selecting ‘Pattern’>’Smoothing’ the following window appears



and the smoothing line will be visualized overlapped to the experimental pattern. The data are smoothed using the Savitzky-Golay filter method (Savitzky & Golay, 1964). The quality of the smoothing can be improved by changing the number of points determining the width of smoothing or modifying the degree of the polynomial function.

K-alpha2 Stripping

http://www.ba.ic.cnr.it/softwareic/qualx/data-reduction/k-alpha2-stripping/

Removes the K-alpha2 contribution from the powder diffraction pattern.

References

http://www.ba.ic.cnr.it/softwareic/qualx/data-reduction/references/

Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., Moliterni, A., Rizzi, R. (2015). J. Appl. Cryst. **48**, 598-603.

Altomare, A., Cuocci, C., Giacovazzo, C., Moliterni, A., Rizzi, R. J. Appl. Cryst. (2008). **41**, 815-817.

Bruckner, S. (2000). J. Appl. Cryst., **33**, 977-979.

Dong, C., Wu, F., Chen, H. (1999). J. Appl. Cryst., **32**, 850-853.

Grazulis, S., Chateigner, D., Downs, R.T., Yokochi, A.F.T., QuirÃ³s, M., Lutterotti, L., Manakova, E.,Butkus, J., Moeck, P. & Le Bail, A. (2009). J. Appl. Cryst. **42**, 726-729.

Grazulis, S., Daskevic, A., Merkys, A., Chateigner, D., Lutterotti, L., QuirÃ³s, M., Serebryanaya, R.N.,Moeck, P., Downs, R.T., Le Bail, A. (2012). Nucleic Acids Res. **40** (Database Issue), D420-D427.

ICDD (2003). The Powder Diffraction File. International Center for Diffraction Data, 12 Campus Boulevard, Newton Square, Pennsylvania 19073-3273, USA.

Madsen, I.C., Scarlett, N.V.Y., Cranswick, L.M.D. & Lwin, T. (2001). J. Appl. Cryst. **34**, 409-426.

Savitzky, A. & Golay, M.J.E. (1964). Anal. Chem., **36**, 1627-1639.

Scarlett, N.V.Y., Madsen, I.C., Cranswick, L.M.D., Lwin, T., Groleau, E., Stephenson, G., Aylmore, M. & Agron-Olshina, N. (2002). J. Appl. Cryst. **34**, 383-400.6

Search

http://www.ba.ic.cnr.it/softwareic/qualx/search-match/

- Database
- Search Match
- Restraints

Database

http://www.ba.ic.cnr.it/softwareic/qualx/search-match/database/

QualX is able to inquire two databases:

1. the PDF-2 commercial database in ASCII format file (pdf2.dat) from which QualX creates the corresponding SQLite database;
2. the POW_COD database (freely available), an SQLite database file created by using the structure information contained in the Crystallography Open Database (COD). A subset of POW_COD database, concerning only inorganic compounds, is also available (POW_COD_INO database).

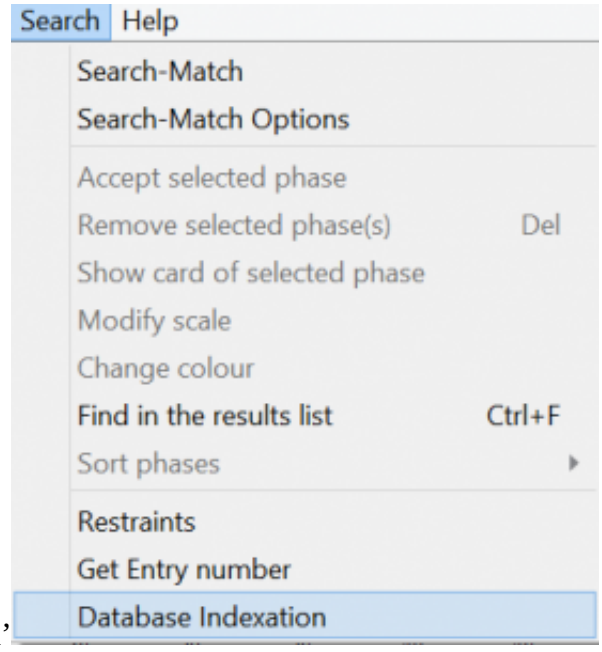
Installation of POW_COD (or POW_COD_INO) database

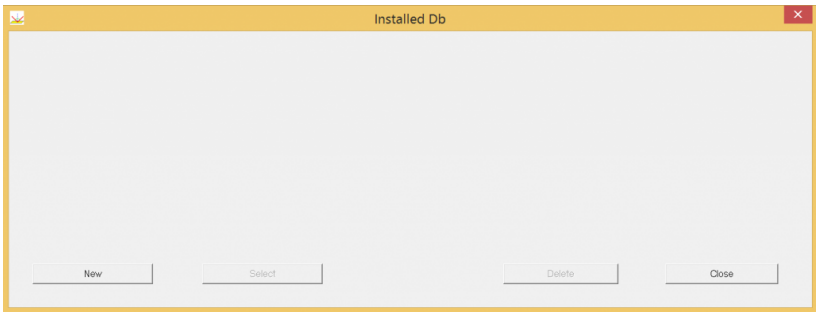
In order to install the POW_COD database:

a. download the POW_COD *.sq file(s) from http://www.ba.ic.cnr.it/content/qualx-downloads. The *.sq files are distributed as single zip file or as five splitted zip files.
b. create a directory where you want to put the POW_COD database.
   In case of single zip file, copy it in the directory and extract it here.
   In case of splitted version:

   i. put in the directory all the five files with extension *z01*, *z02*, *z03*, *z04* and *zip*;
   ii. extract only the file identified with extension *zip*, the other zip files will be automatically extracted
   (please note that extracted files have to be left in the same folder).

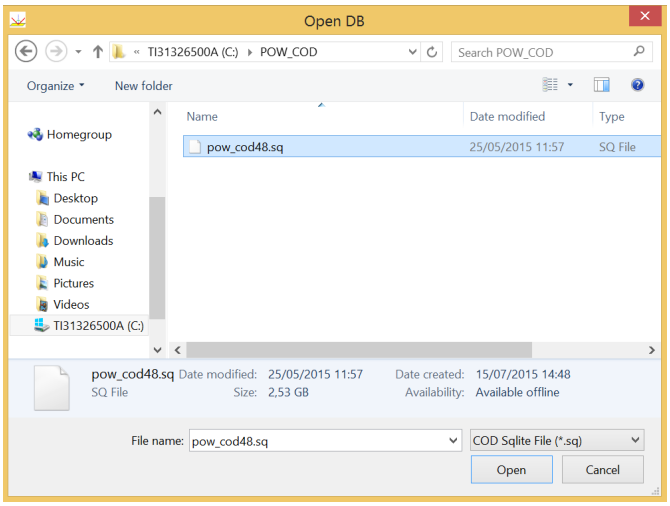
3. run QualX
4. Select ‘Search’ >’Database Indexation’



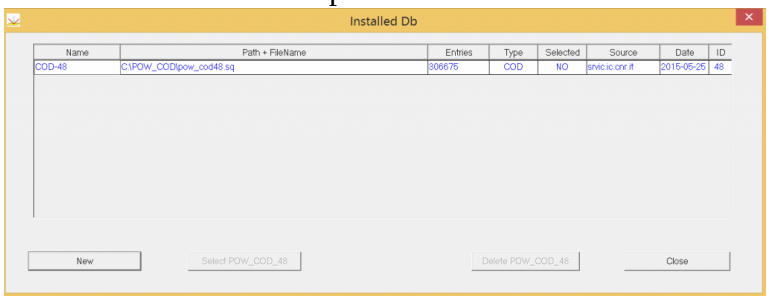


5. Click on the button ‘New’ , a window will be opened enabling to select the directory containing the

   The following window will appear:

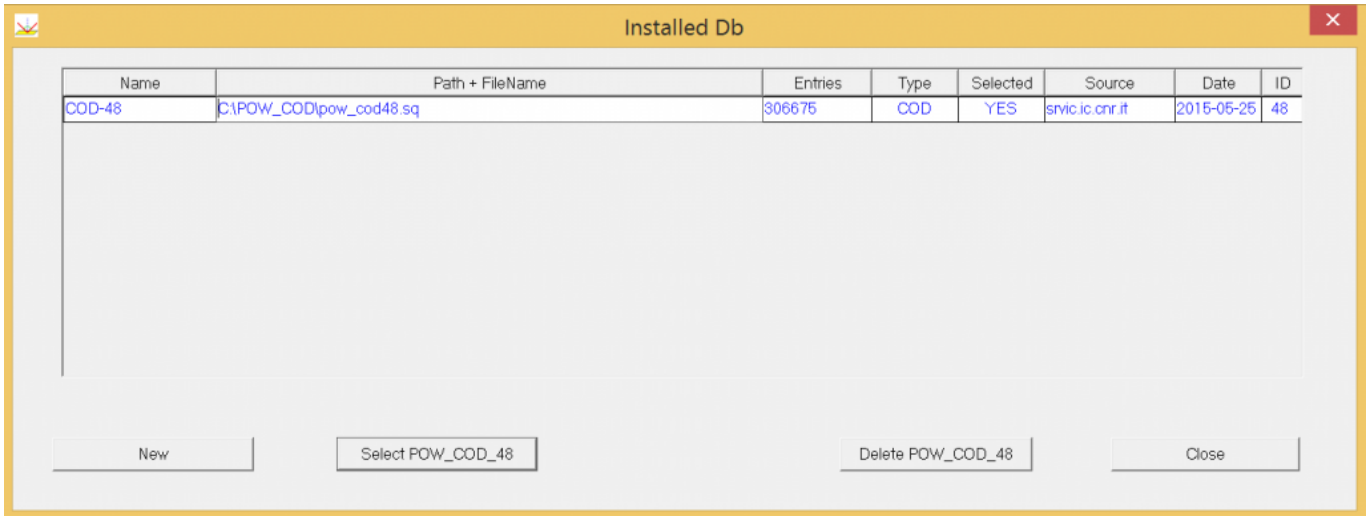


Once the POW_COD database file has been selected click on ‘Open’ .??



select the corresponding row in the window by left click of the mouse.

7. To make active the database in the search click on ‘Select POW_COD_XX’ (‘YES’ will appear in
the ‘Selected’ column) and then on’Close’ .



POW_COD database file (i.e., pow_cod48.sq).

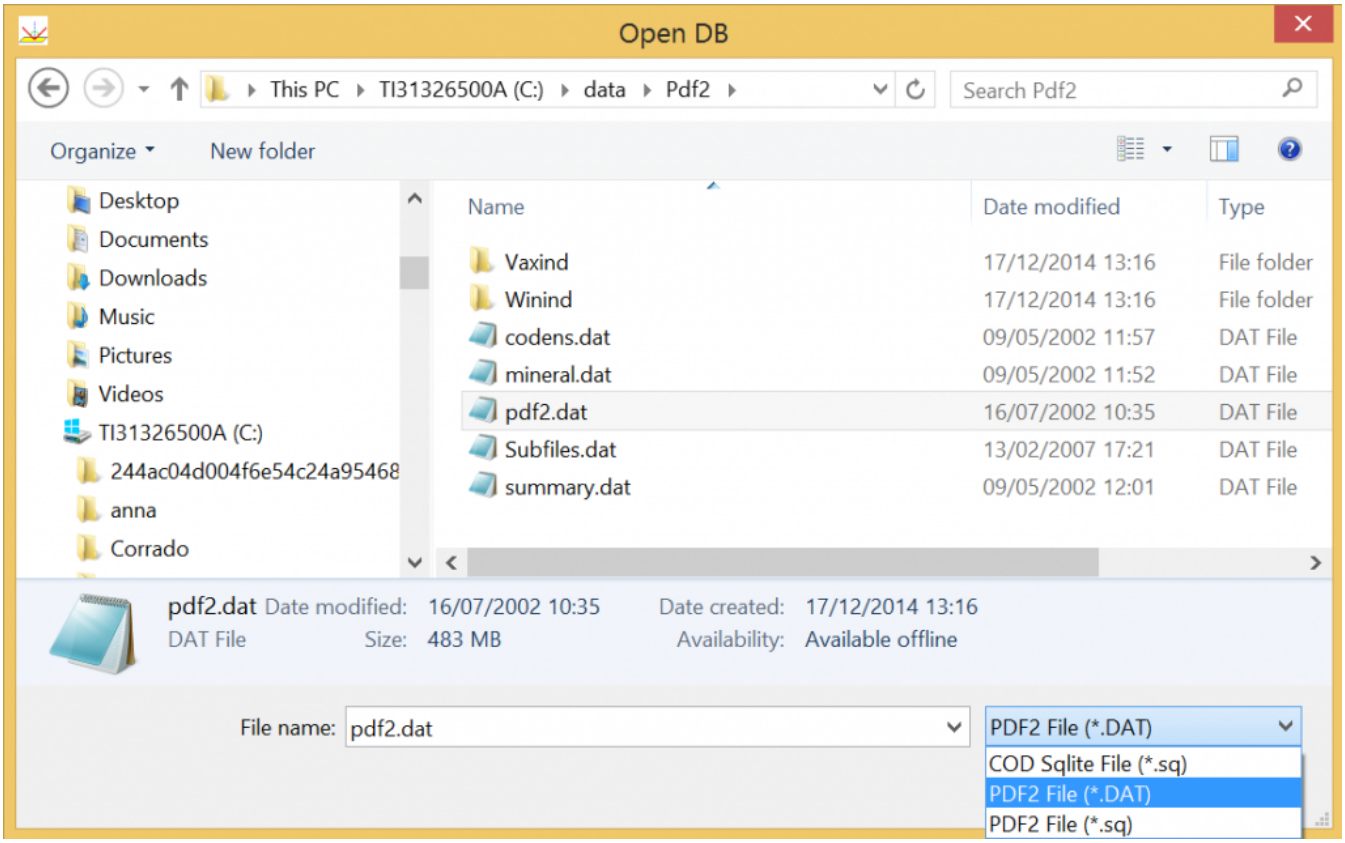
A similar procedure has to be followed in case of the database concerning only inorganic compounds (POW_COD_INO); in this case

1. download the POW_COD_INO database single zip file.

2. create a directory where you want to put the POW_COD_INO database, copy the single zip file in the directory and extract it here.
3. repeat the steps c)-g).

Installation of PDF-2 database

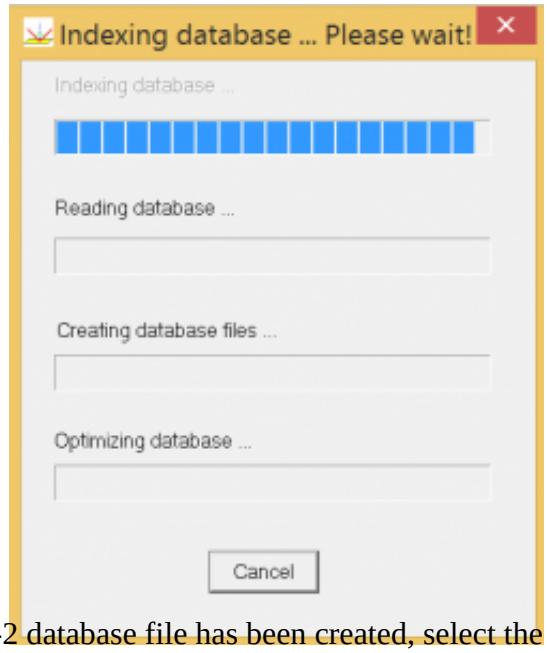
If the PDF-2 database (PDF-2 Release 2004 or earlier versions) is available on your PC, it can be installed by the following instructions:
1) the points c)-e), described to install the POW_COD database, must be repeated; at step e), select the directory containing the PDF-2 database



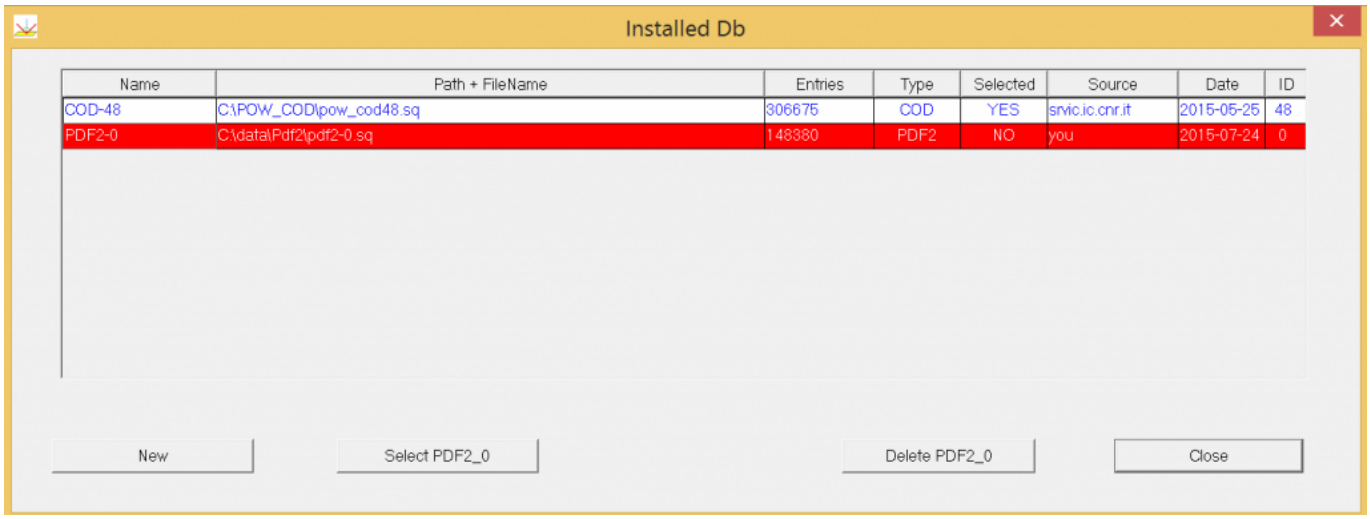
select the ASCII file ‘pdf2.dat’ and click on ‘Open’ to generate the corresponding SQLite database.

The files ‘codens.dat’, ‘mineral.dat’ and ‘summary.dat’ are also required by QualX so it is strictly suggested to copy and leave the folder containing these files on your hard disk;

2) The installation of PDF-2 database can take several minutes.
The following window showing the progress of the database indexation will appear;



3) Once the PDF-2 database file has been created, select the row concerning it



click on the corresponding selection button ‘Select PDF2_X’ (‘YES’ will appear in the ‘Selected’ column) and finally click on ‘Close’ .

Search Match

http://www.ba.ic.cnr.it/softwareic/qualx/search-match/search-match/

The selection ‘Search’>’Search-Match’ enables the search of database reference patterns best matching the experimental powder diffraction data. At the end of the search-match step, QualX provides a list of plausible phases sorted according to a decreasing Figure of Merit (FoM) calculated by taking into account the number of matched peaks, the average difference in peak position and the average difference in peak intensity between the observed and database lines.

The value of FoM is given by the following formula:

$$FoM = \sqrt{\frac{FoM_{db} \cdot \left(w_{\theta} \cdot FoM_{\theta} + w_{I} \cdot FoM_{I} + w_{ph} \cdot FoM_{ph} \right)}{w_{\theta} + w_{I} + w_{ph}}}$$

including four different agreement contributions FoM_{db}, $FoM_{?,}$, FoM_{I}, FoM_{ph} and the weighting factors $w_{?,}$, w_{I}, w_{ph}.
$FoM_{?,}$ is the contribution coming from the 2?¸ differences between the experimental and the associated database peaks:

$$FoM_{\theta} = 1 - \frac{\sum_{i}^{N_{db}^{ass}} |2\theta_{i}^{\exp} - 2\theta_{i}^{db}|}{N_{db}^{ass} \cdot \Delta}$$

where the summation is over the associated database peaks (a database peak is considered associated if its 2?¸ distance from the experimental peak is less then ?), $2?^{exp}$ and $2?^{db}$ 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:

$$FoM_{I} = 1 - \frac{\sum_{i}^{N_{\exp}^{ass}} \left| I_{i}^{\exp} - I_{i}^{db} \right|}{N_{\exp}^{ass}}$$

where I^{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:

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

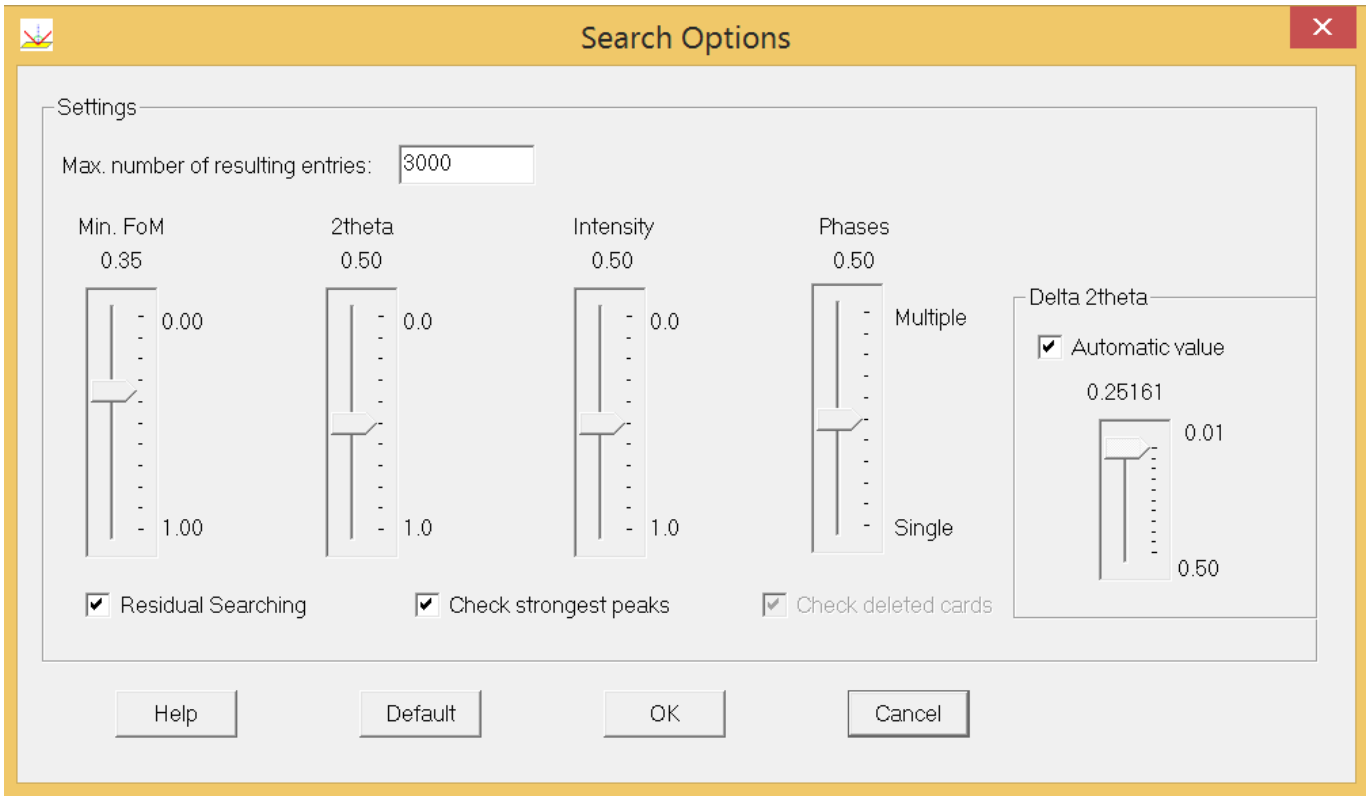
where N_{exp} is the total number of experimental peaks.

FoM_{db} is the contribution due to the intensities of the associated database peaks and their percentage:

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

where I_{db} is the database intensity and the summation at the numerator is over the associated database peaks. N_{db} is the total number of the database peaks.
The weighting factors $w_?$, w_I, w_{ph} and ? (default heuristic values for them are set) can be adjusted directly by the user by using the graphical interface. w_{ph} is related to the number of expected phases.
The search-match parameters can be modified selecting ‘Search’>’Search-Match Options’ and changing the fields in the following window.

Search Options Dialogue:



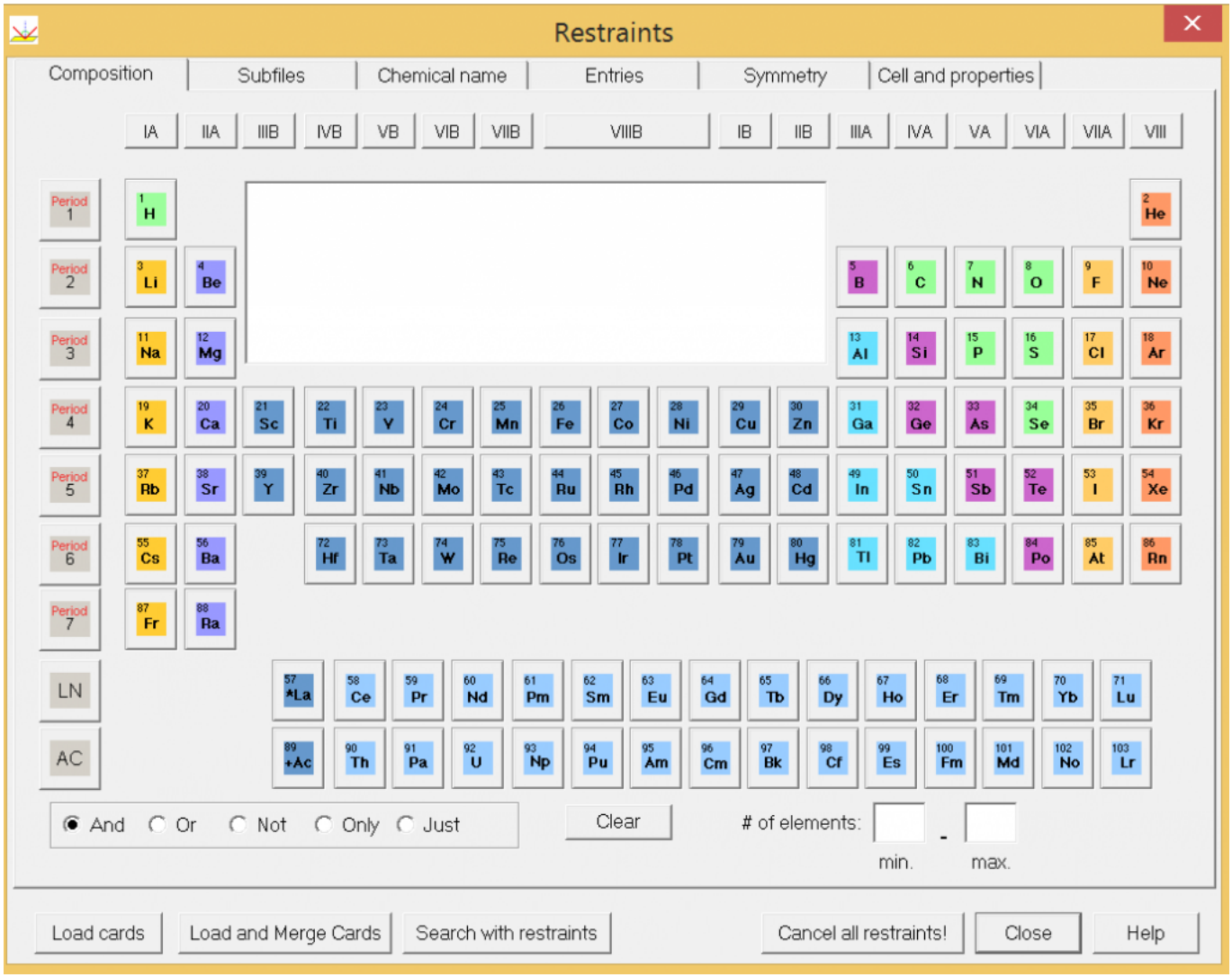
Max. numbers of resulting entries: modifies the maximum number of entries with the highest FoM that can be shown at the end of the search-match step. The maximum number of entries that can be visualized in the results list is 8000.
Min. FoM: selects the minimum value for the figure of merit. All entries with FoM lower than “Min. FoM” will be not considered and not shown in the results list at the end of the search-match step.
2theta: sets the weight ($w_?$) of the peak positions contribution in the FoM calculation. 1.0 means that the agreement between the experimental peak positions and those ones of the database entry matched lines strongly influences the FoM value.
Intensity: sets the weight (w_I) of the peak intensities contribution in the FoM calculation. 1.0 means that the agreement between the experimental peak intensities and those ones of the database entry matched lines strongly influences the FoM value.
Phases: sets the weight (w_{ph}) related to the expected number of phases in the sample. “Single” has to be selected if only one phase is expected.
Residual Searching: if this option is active (default choice), as soon as a candidate entry in the results list is accepted, its contribution is subtracted from the list of experimental (d,I) values, obtaining an updated set of (d,I). For the rest of candidate entries the FoM is calculated again by taking into account the updated (d,I) values and the entries are sorted once again in function of the new FoM values. This option can be useful to identify minority phases. If the option is not active the results list will be not modified if a candidate entry is accepted.
Check strongest peaks: if this option is active (default choice), QualX selects as candidate phases the database entries that have at least the N strongest lines ($N=3$) very close (within a certain range) to the experimental d values. This option strongly speeds the search process without losing reliability. If this option is not active the selection of the database entries is based on the rule that at least one d value must be matched.
Check deleted cards: if this option is active, all the entries in the database characterized by a ‘D’

Quality Mark (‘D’ means deleted) are excluded from the search step. The option is activated (default option) only if the PDF-2 database is used.
Delta 2theta: sets the maximum allowed difference between the 2*?* position of an experimental peak and that one of a database entry line, according to which the line can be considered matched. The ‘Automatic value’ is calculated by taking into account the FWHM of the experimental peaks.
In case of presence of very broad (or very narrow) observed peaks, the automatic value of ‘Delta 2theta’ could be too large (or too small). In this case, it can be useful to change the ‘Automatic value’ by deactivating this option and supplying the new value *via* the trackbar.
Default: restores the default settings.

Restraints

http://www.ba.ic.cnr.it/softwareic/qualx/search-match/restraints/

Restraints on Composition



The following boolean operators are available to impose restraints in the search-match step.
And: all the selected chemical elements must be in the resulting phases.

Or: at least one of the selected chemical elements must be in the resulting phases (additional chemical elements can be present).

Not: none of the selected chemical elements must be in the resulting phases.

Only: only the selected chemical elements must be present simultaneously in the resulting phases. *E.g.*, selecting Si and C elements only phases like Si_xC_y will appear in the results list.

Just: all phases containing at least one of selected elements will be in the results list. *E.g.*, selecting Si and C elements only phases *Si*, C_x, Si_yC_z will appear.

Restraints on minimum and/or maximum number of chemical elements can be imposed using the following entries

Press button CLEAR to cancel restraints.

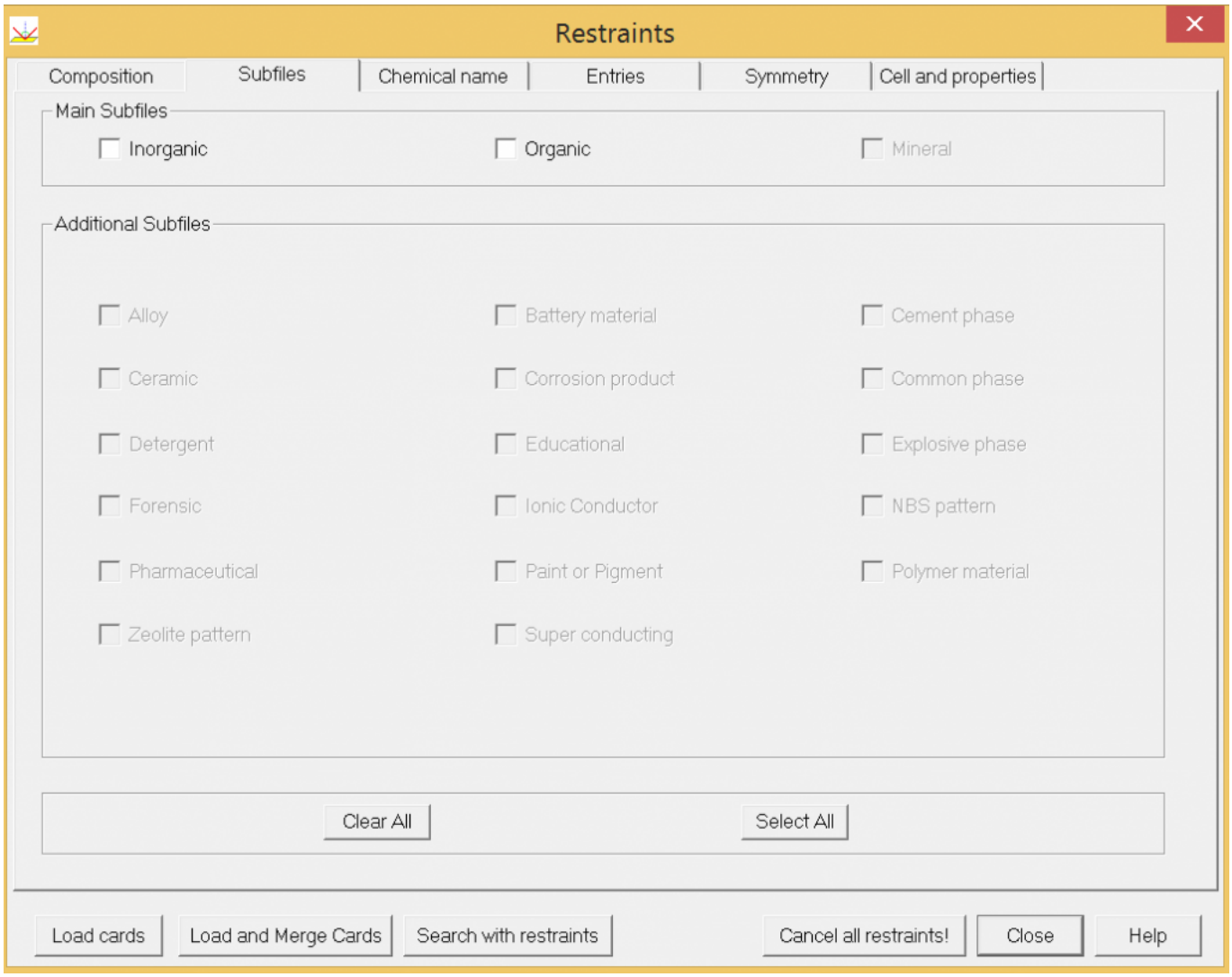
Load Cards: only the phases that satisfy the restrictions will be shown in the results list;

Load and Merge Cards: if the search-match step has been already performed, the new entries satisfying the restrictions will be combined with the entries already listed;

Search with restraints: the search-match step is executed using the imposed restraints;

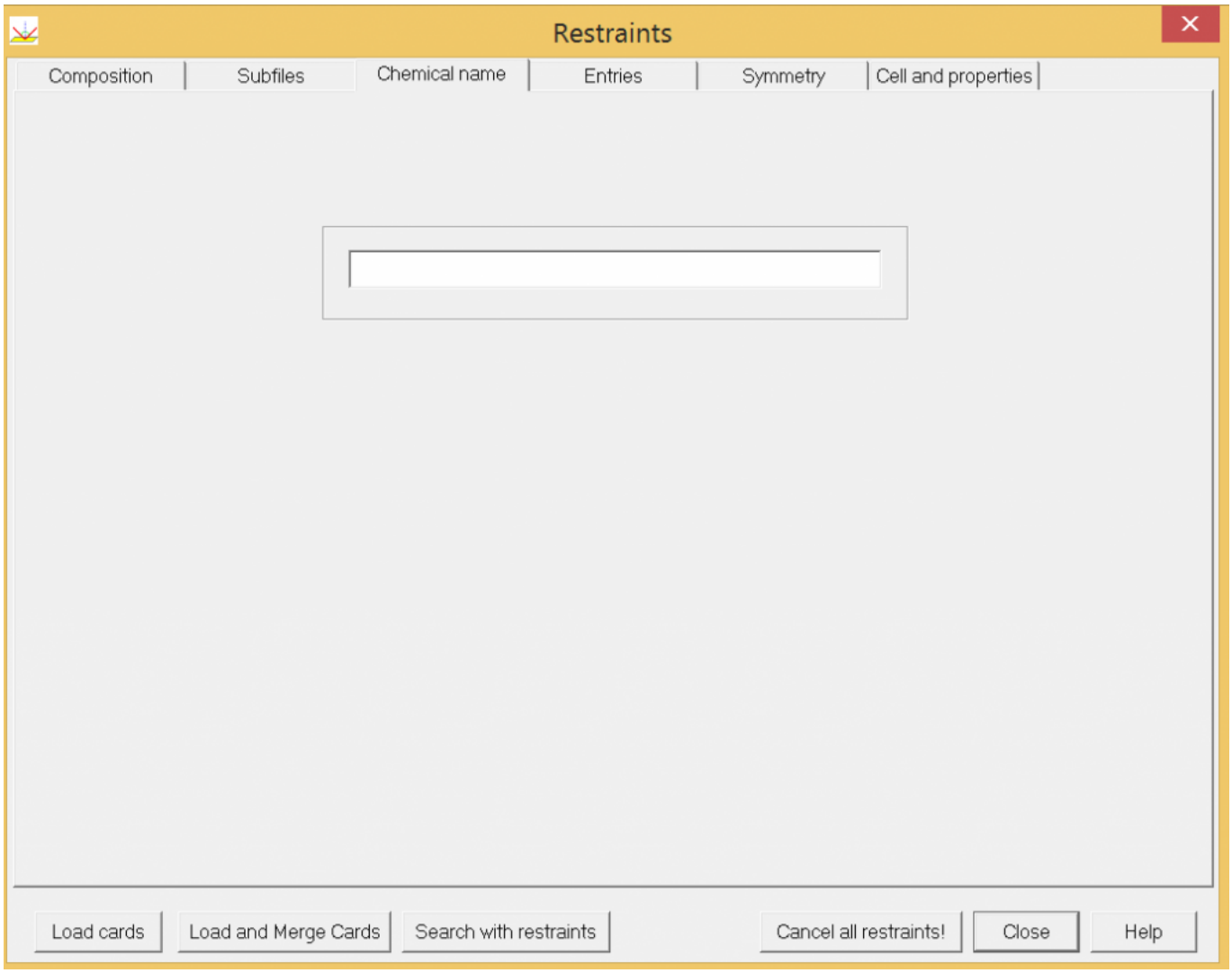
Cancel all restraints: all the imposed restraints are deleted.

Restraints on Subfiles



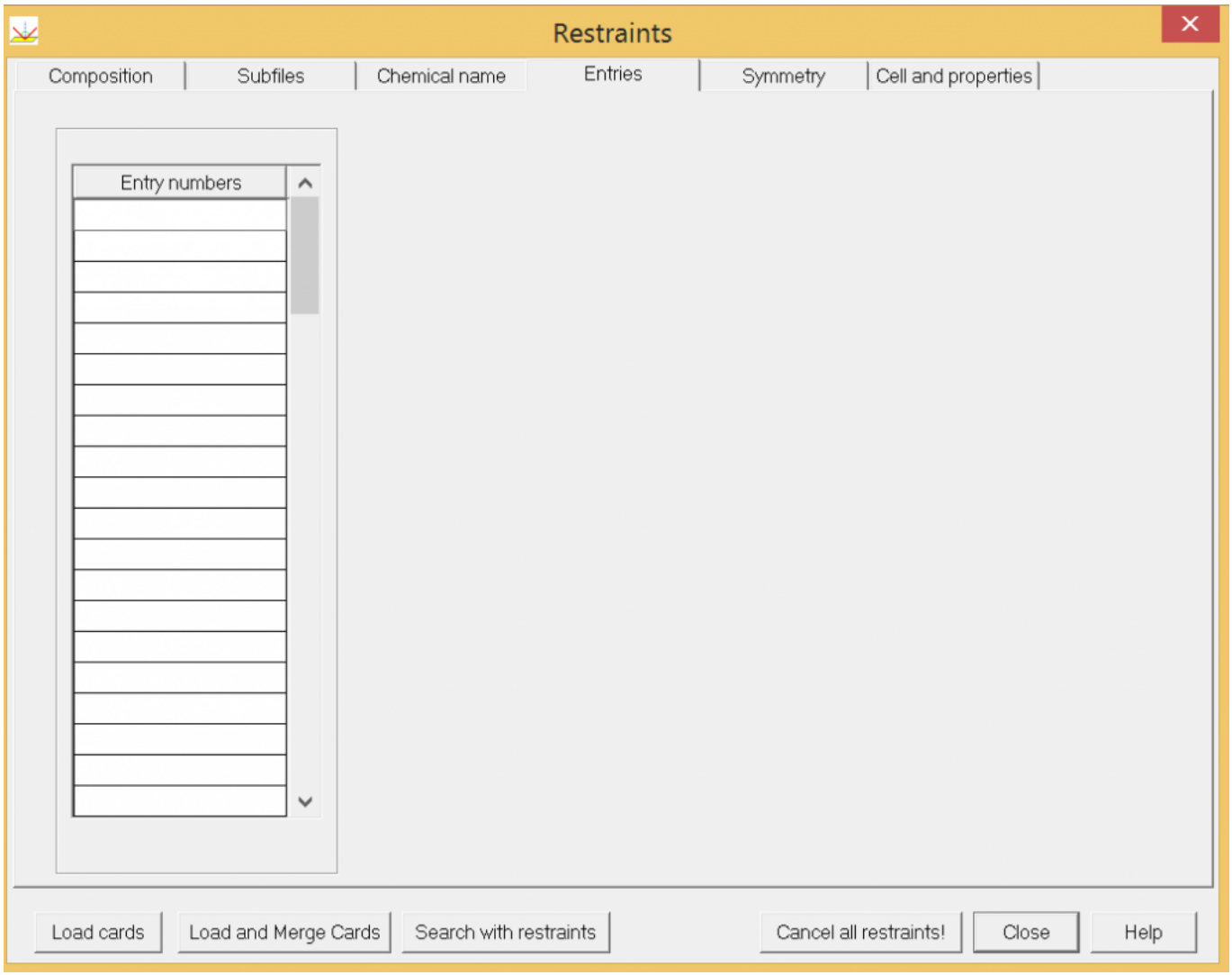
To limit the search to one or more than one selected class of compounds.

Restraints on Chemical name



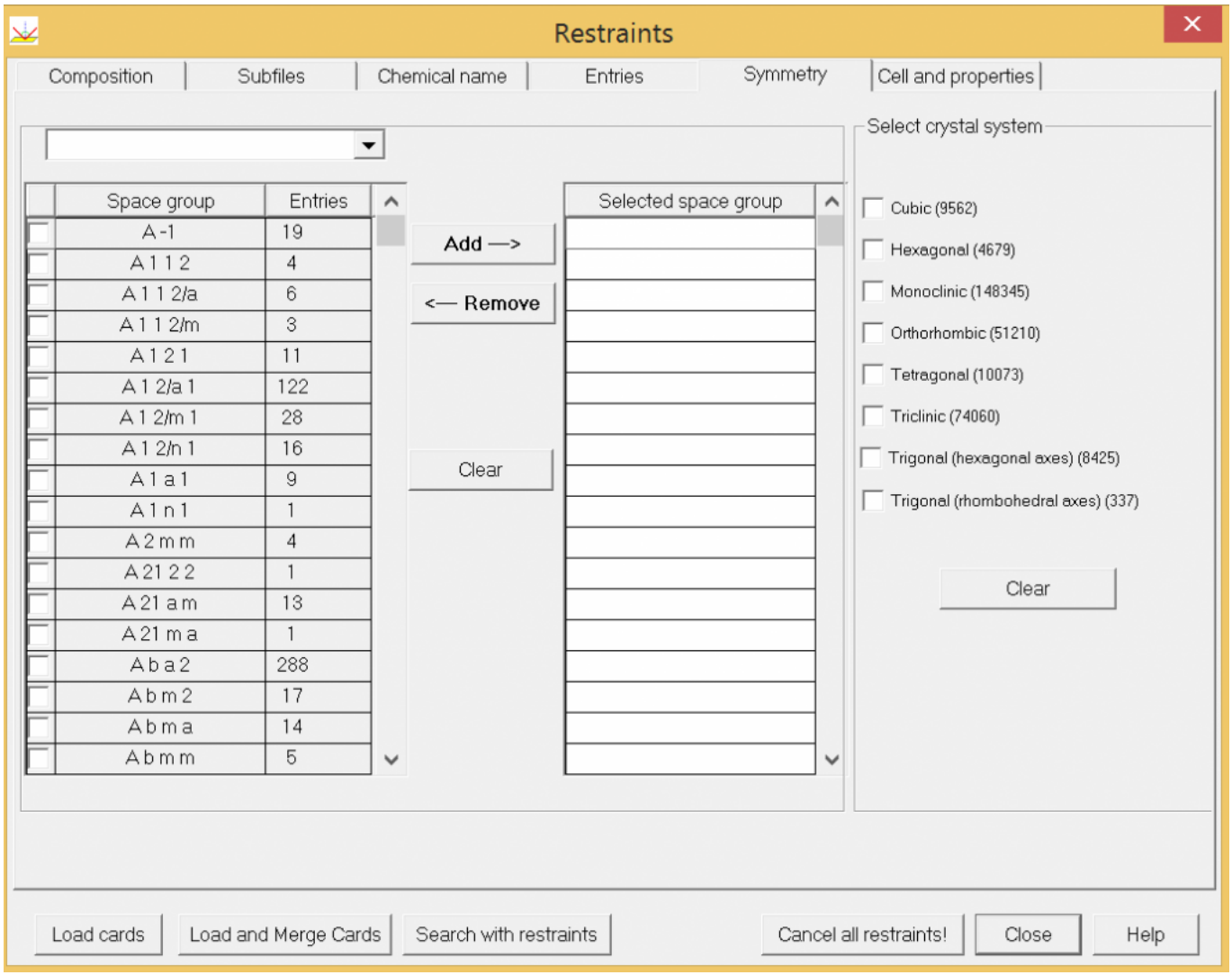
The search is limited to phases with compound name containing the string supplied in the entry box.

Restraints on Entries



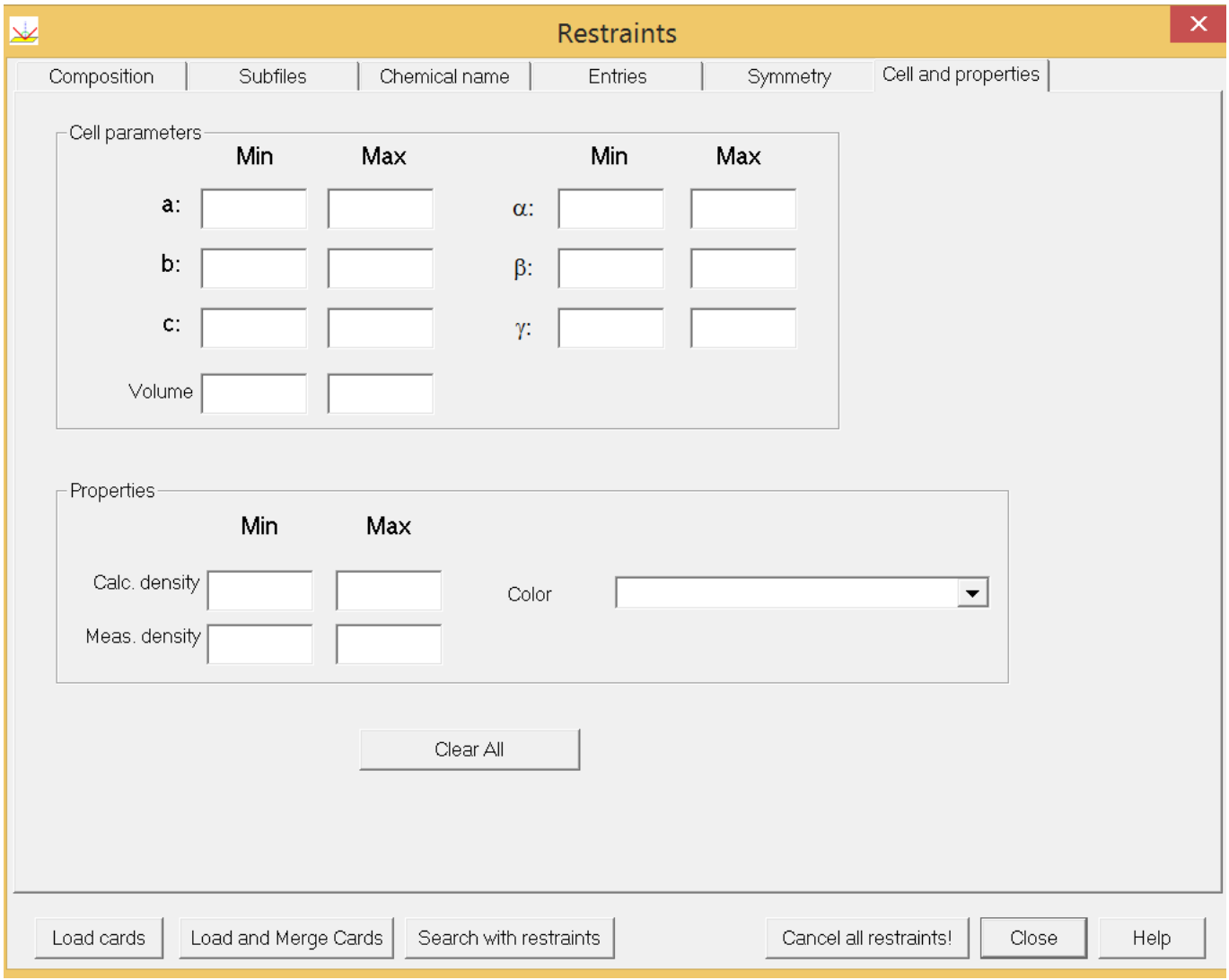
?The search is limited to phase(s) corresponding to the typed entry number(s).

Restraints on Symmetry



The search is limited to phase(s) whose space group and/or crystal system have been selected by check button.
In case of restraints on space group(s), the restraints selection (or removal) is executed by clicking on ‘Add’  (or ‘ Remove’ ) button.
The ‘Selected space group’ column contains the list of space group(s) selected and actively used in the Restraints.
The restraints on ‘Symmetry and on ‘Cell and properties’ could be not applicable if an old version of the database is used.

Restraints on Cell and properties



?The search is limited to phase(s) characterized by cell parameters, and/or cell volume, and/or calculated density and/or measured density lying in the user supplied range of values. Restraints on crystal color can be set also; in case of POW_COD database the available list of colors is the collection of the crystal color descriptions supplied in the COD CIF files corresponding to the POW_COD entries.

Graphic options

http://www.ba.ic.cnr.it/softwareic/qualx/graphic-options/

- Graphic area
- File
- View
- Pattern
- Search
- Help

Graphic area

http://www.ba.ic.cnr.it/softwareic/qualx/graphic-options/graphic-area/

The graphic area of QualX program is composed by 3 parts:

powder pattern area: visualizes the powder pattern on top at left.

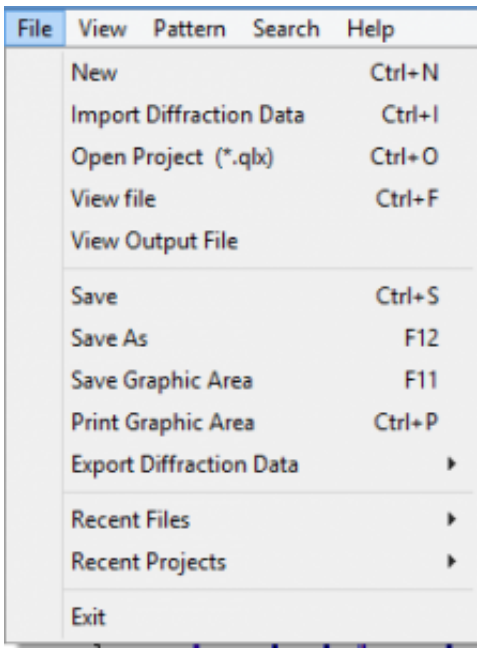
peak list area: it is a grid on top at right containing the peak list of the experimental pattern, the accepted and selected phases. Selecting one or more peaks in the grid the corresponding peak(s) in the pattern is (are) marked. Clicking on the button  and pulling the mouse on the powder pattern area it is possible to highlight peaks on the grid. If you press ‘Delete Peaks’ in the menu ‘Pattern’ the selected peaks will be deleted.

results list: shown in the lower part of the window, it contains information about the phases obtained after the search-match step. Some information will appear: the quality mark (QM); the entry number (CARD); the compound name; the chemical formula; some of the contributions to the total FoM concerning peak positions (‘Peakpos.’ column) and intensities (‘Intensity’ column); the scale value; the total FoM (‘FoM’ column); the I/Ic value useful for a semi-quantitative analysis (‘S-Quant.’ column). The check bottons in the last column allow to keep visible more than one phase in the powder pattern area.
Use the button ‘Remove selected phase(s)’ in the menu ‘Search’ to delete the selected phase (by mouse click). A group of phases can be deleted but they must be selected by the mouse.

File

http://www.ba.ic.cnr.it/softwareic/qualx/graphic-options/file/

File Menu



New: resets the graphic area, list of results, peak list, stack for undo/redo. 

Import Diffraction Data: loads the pattern from file. The program can manage only the following file types:

1. **ASCII file (start, step, end, intensities)**: The first row contains 2*?* minimum, 2*?* step, 2*?* maximum. Counts are in the successive lines. The number of counts for row or the format of counts can vary

```
# example 1 for ascii file with start,step,end, intensity
6 0.020 90.0
149. 161. 151. 136. 144. 151. 150. 149. 117. 138.
157. 120. 143. 156. 110. 142. 147. 147. 124. 128.
130. 144. 134. 159. 145. 150. 138. 149. 134. 159.
142. 139. 135. 136. 147. 139. 155. 133. 140. 133.
134. 158. 165. 134. 156. 139. 122. 141. 158. 132.
150. 138. 134. 149. 147. 150. 154. 165. 145. 140.
.................................................
# example 2 for ascii file with start,step,end, intensity
6.0 0.010 70
79 58 76 73 80 73
```

```
68 72 93 66 67 60
72 83 65 72 87 76
78 73 65 83 77 75
95 127 138 175 206 208
176 170 126 124 96 82
67 66 71 68 72 74
116 123 89 123 141 131
137 116 113 82 84 65
70 81 82 89 119 146
.................................................
```

2. **ASCII file (2 columns: 2theta and intensity)**: this file contains 2*?* in the first column and intensities in the second one. The format can vary.

```
# example for ascii file with 2 columns
3.0000 96.750
3.0200 96.500
3.0400 83.000
3.0600 94.000
3.0800 87.000
3.1000 94.000
3.1200 93.000
3.1400 75.750
3.1600 84.250
3.1800 76.500
3.2000 83.250
3.2200 78.750
3.2400 75.500
.................................................
```

Use symbol '#' to introduce comment lines.

3. **Additional readable ASCII file formats are: GSAS (**.gda*), CIF (**.rtv, *.cif*) and XYE (**.xye*).**

Open Project (*.qlx): opens a project created by QualX  .

View file: visualizes a text file.

View Output File: visualizes the output file in html format.

Save: saves all changes in the project previously created. 

Save As: saves all changes in a new project.

Save Graphic Area: exports the powder pattern area in a file.

Print Graphic Area: prints the powder pattern area.

Export Diffraction Data: by this option it is possible to export the diffraction pattern in two of the possible formats managed by QualX (file type 1. and 2. previously described). By selecting ‘Peak data’ it is also possible to save the *(d,I)* values [or the *(2?,I)* values] associated to the experimental peaks in an external file (two columns file).

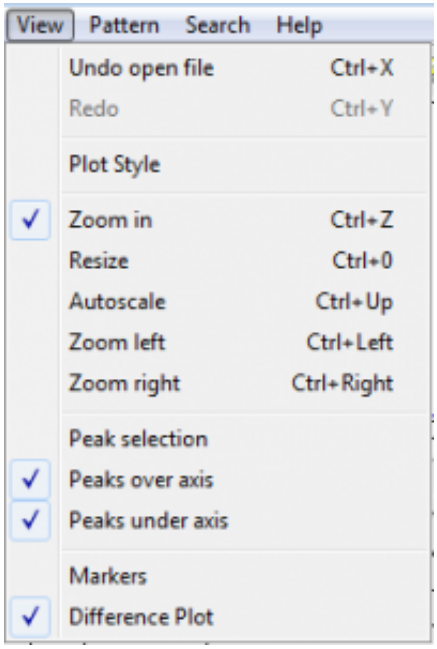
Recent Files: list of the last five recent files.

Recent Projects: list of the last five recent projects.

View

http://www.ba.ic.cnr.it/softwareic/qualx/graphic-options/view/

View Menu



Undo/Redo: Use undo option to erase the last operation. The redo option reverses the undo one. 

Plot Style: opens a window to modify colours and styles of the graphic area.

Zoom in: enables the zoom. When the zoom is enabled the cursor appears as a magnifying glass. 

Resize: shows the complete pattern if a zoom of the pattern has been carried out. 

Autoscale: rescales the plot up to the highest intensity in the zoom area. 

Zoom left: moves to the left the zoom area. 

Zoom right: moves to the right the zoom area. 

Peak selection: tags the peaks in the area of the pattern selected by mouse. 

Peak over axis: visualizes peaks with long bars over the X axis. 

Peak under axis: visualizes peaks with short bars under the X axis. 

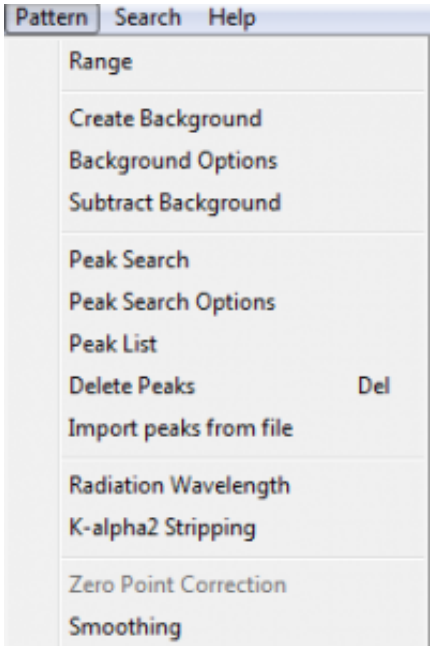
Marker: enables the visualization of powder pattern with markers. 

Difference Plot: enables the visualization of differences between experimental peak intensities and line intensities of the selected phase. 

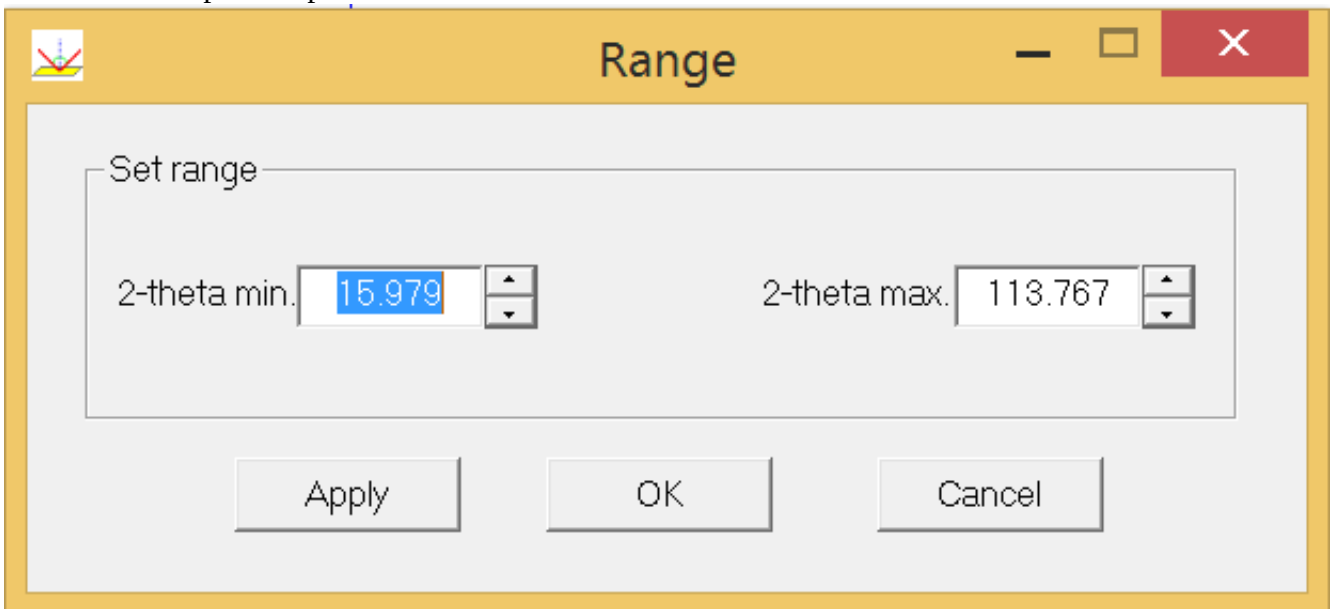
Pattern

http://www.ba.ic.cnr.it/softwareic/qualx/graphic-options/pattern/

Pattern Menu



Range: opens the following dialogue window to modify the minimum 2? value and/or the maximum 2? value of the powder pattern.



Edit the new limits or use the mouse to move the two vertical bars setting the 2q range.

Create Background: creates automatically the background and shows it.

Background Options: opens dialogue window to manually modify the background. Select this button when the automatic background is not well estimated.

Subtract Background: after the creation of background, select this button to subtract background from the pattern.

Peak Search: performs an automatic peak search.

Peak Search Options: modifies the peak search options. By clicking on the bottom  the peaks can be added or removed manually (by left or right click of mouse).

Peak List: shows a list of peaks.

Delete Peaks: deletes selected peaks.

Import peaks from file: imports a list of peaks from external file containing the d values (or 2q values) and relative intensity values.

Radiation Wavelength: sets the radiation wavelength.

K-alpha2 Stripping: carries out the K-alpha2 stripping.

Zero Point Correction: select this option to calculate the zero point shift

Smoothing: press this button to carry out the powder pattern smoothing

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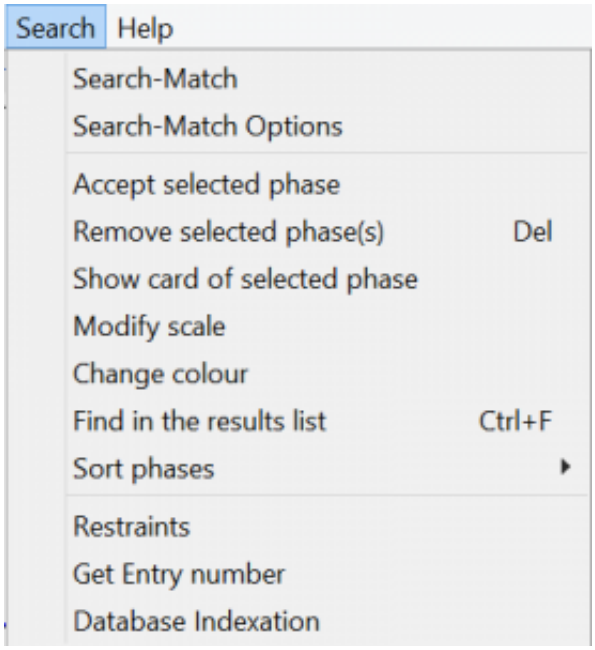
Search

http://www.ba.ic.cnr.it/softwareic/qualx/graphic-options/search/

Search Menu



Some options of this menu are quickly activated via the buttons shown on the right in the following figure:

Search-Match: performs the search-match step. The restraints supplied via the restraints window will be actively used during the search.

Search-Match Options: opens window to modify the search options. 

Accept selected phase: accepts the selected phase. The accepted phase will be highlight in yellow at the top of list. Use this button to remove phases from the list of accepted phases (list of yellow phases).


Remove selected phase(s): removes a phase from the results list. A group of phases can be deleted (they must be selected in the results list by mouse).

Show card of selected phase: shows the card of the selected phase. 

Modify scale: the program automatically rescales the peak intensities of the reference pattern by taking into account the associated peaks in the experimental pattern. Use this button to modify the scale value.

The FoM value will be updated. 

Change colour: changes the colour automatically assigned by QualX to each entry in the results list. 

Find in the results lists: to find, in the results list, a string typed in the entry box. 

Sort phases: as default choice, the phases are sorted according to the total FoM but via the ‘Sort phases’ option it is possible to modify the order using a different column as key.

Restraints: opens window to set restraints.

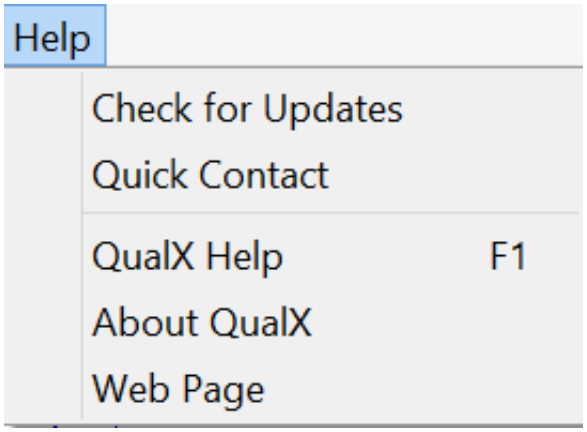
Get Entry number: gets entry from the ID number (*e.g.*, 00-034-0427 or 000340427 or 340427)

Database Indexation: installs a database.

Help

http://www.ba.ic.cnr.it/softwareic/qualx/graphic-options/help/

Help Menu



Check for Updates: checks if the current version of QualX is the latest one.

Quick contact: to send a message to the authors.

QualX Help: accesses to QualX help file.

About QualX: gets general information about QualX (version, build data, authors, contacts).

Web page: link to the QualX Web page.

Qualx2

a qualitative phase analysis software