iQual: a qualitative phase analysis software

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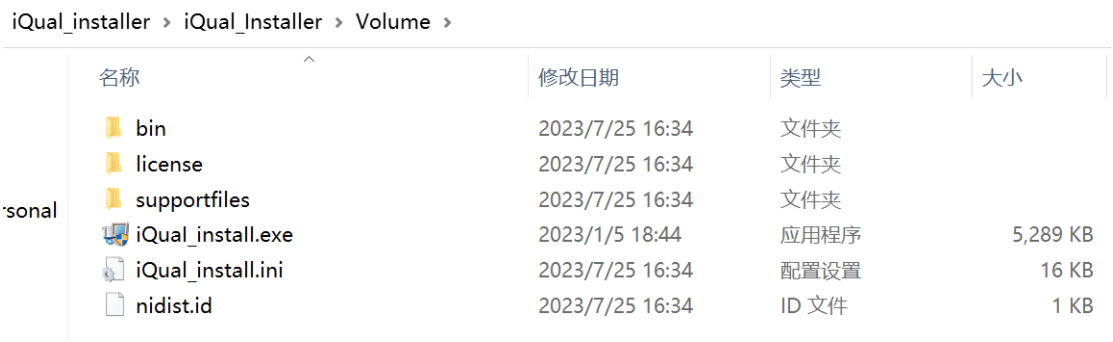
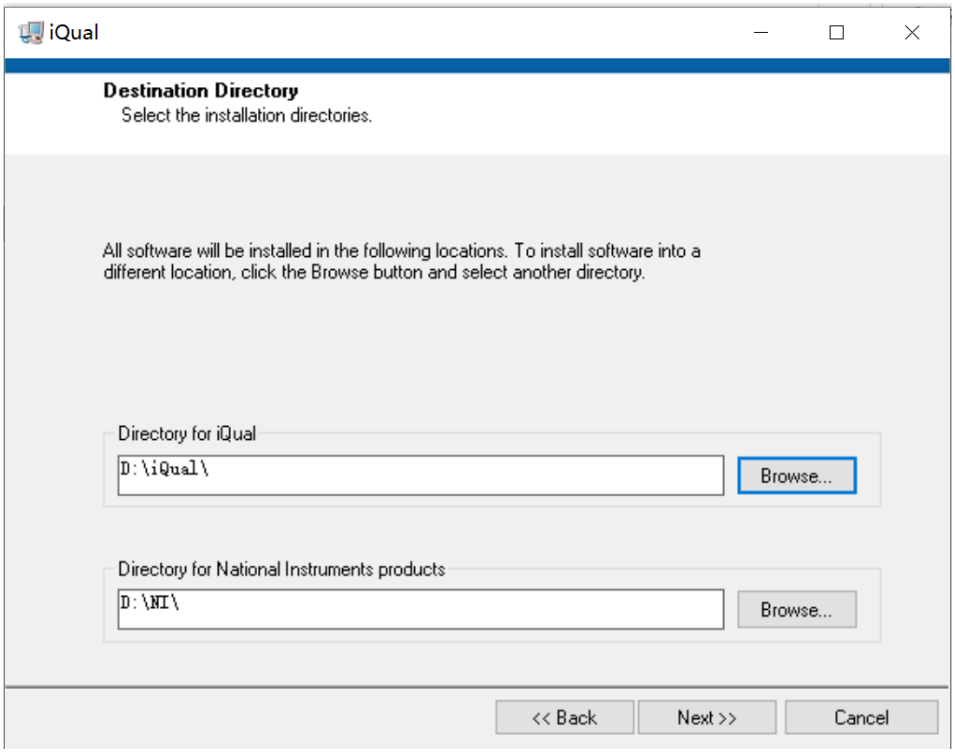
Installation:

First of all, please download iQual-install.zip, python.zip and Crystal_db.zip, and unzip them. You can download them from GitHub (https://github.com/iPowder/iQual and https://github.com/iPowder/Crystal_db) or WorkDrive (https://workdrive.zohopublic.com.cn/folder/bgee25b186e54186b4970972866057796b23be).

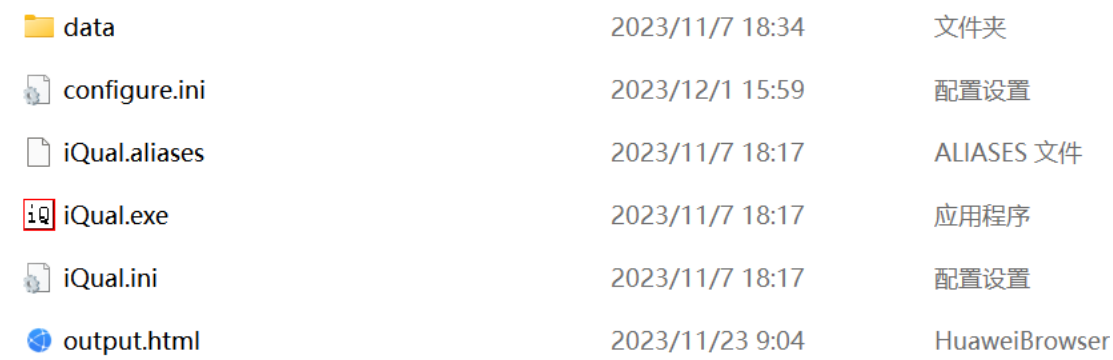
1. Install iQual by clicking iQual_install.exe in the unzipped file folder.



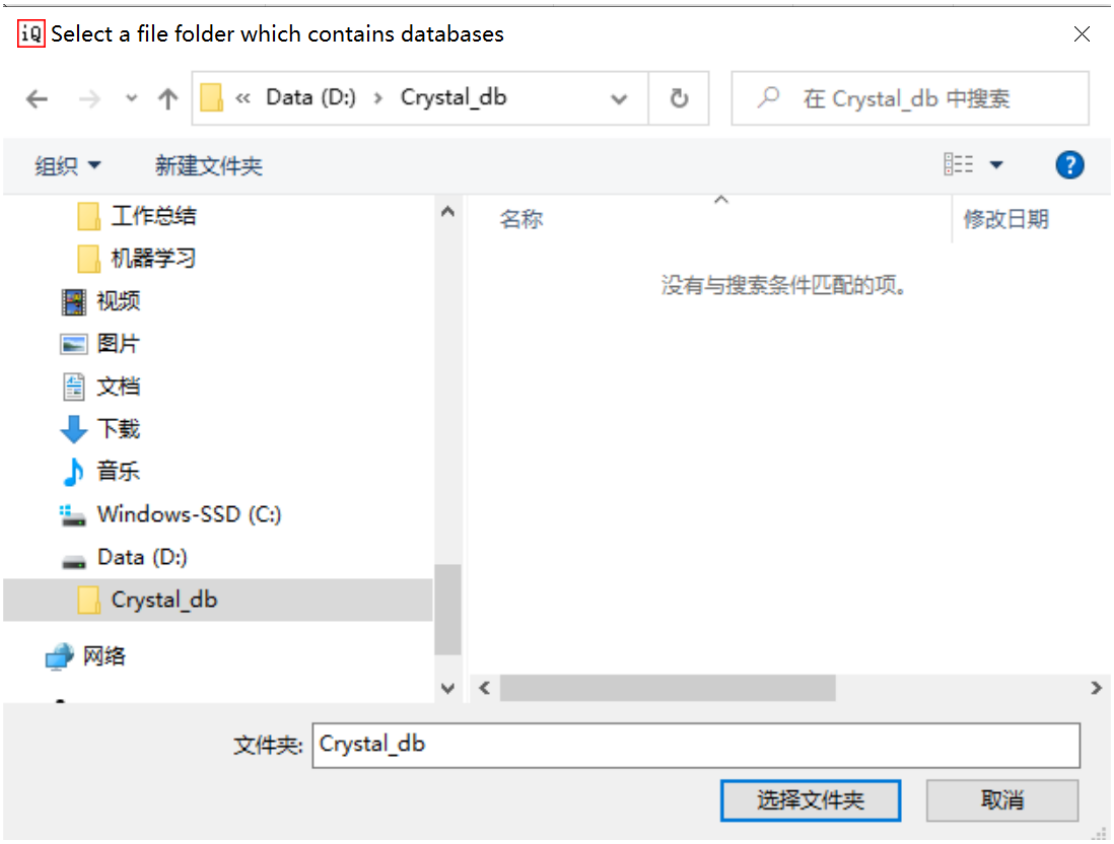
2. Choose two empty file folders (cannot contain Chinese characters) to install iQual and LabVIEW dependency.



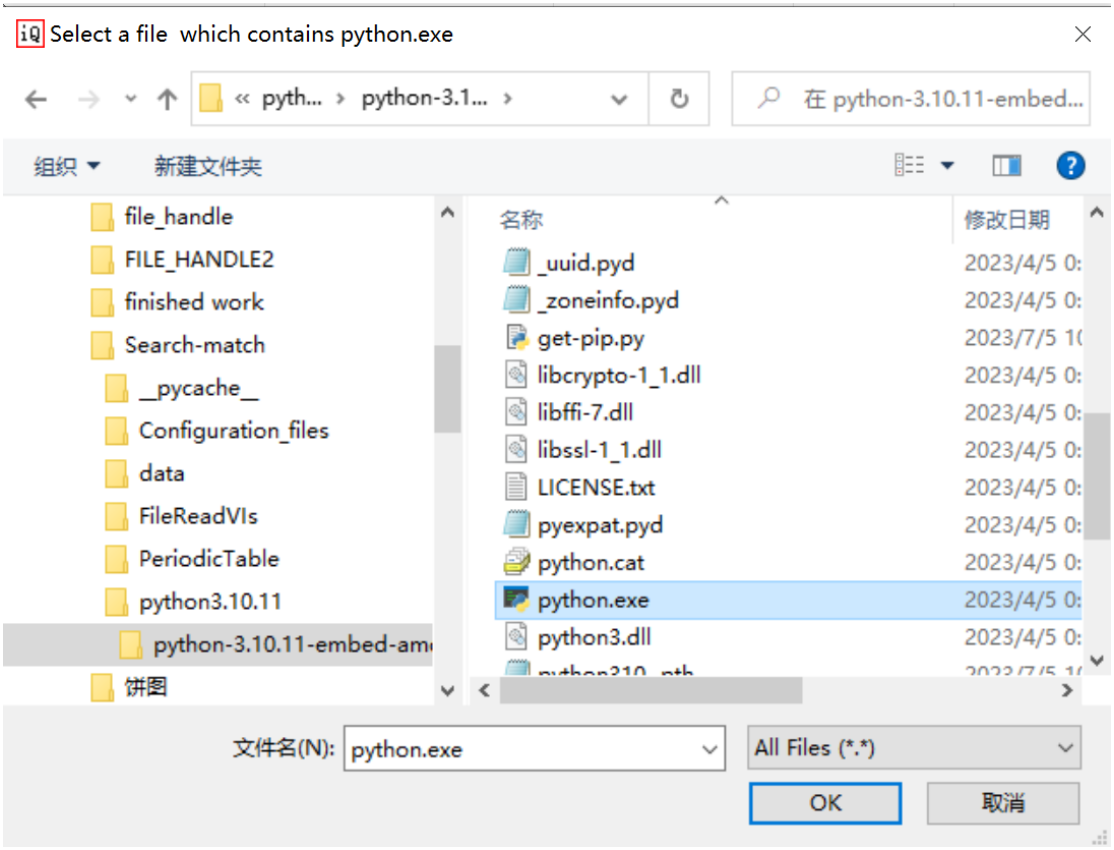
3.You can find the program in the installation path, start the program by click iQual.exe .



4.When the program is started at first time, it will pop a file folder window for user to choose a folder with the database files and python.exe file which is in python.zip you have downloaded. This is because the configure file which contain the database path is empty or not exists (/iQual/configure.ini).



Then,



Then we can see the settings in the configure.ini file:

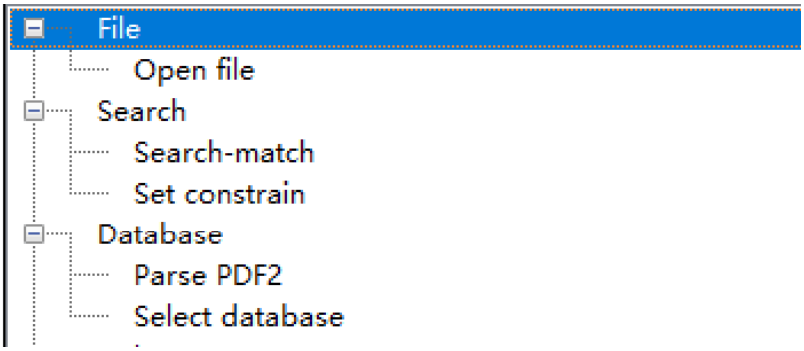
```
[database]
path = "D:/Crystal_db/"

[python]
path = "D:\\python-3.10.11-embed-amd64\\python.exe"
```

Quick start

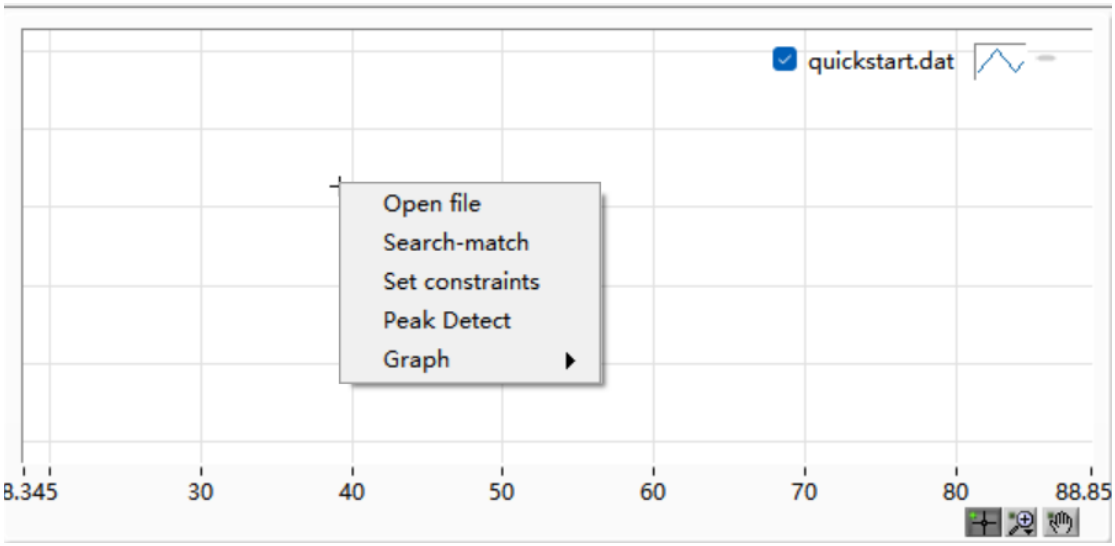
1. Open a file by clicking “Open file” in main menu or right clicking “Open file” in the graph menu.

Main menu: File Search Database Help

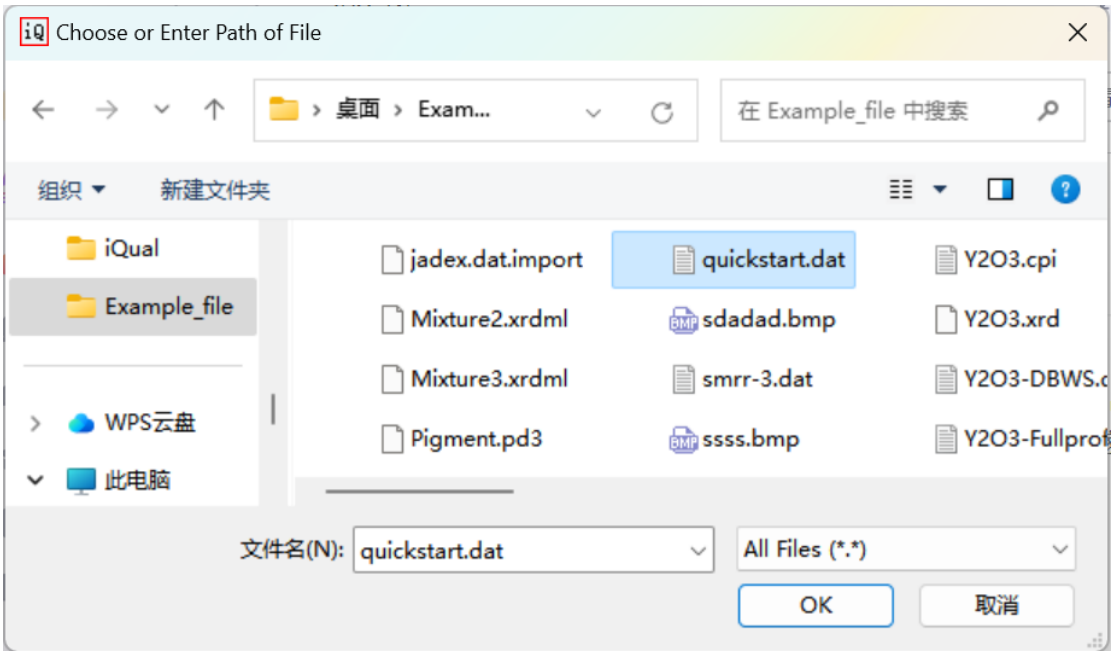
Main menu structure:



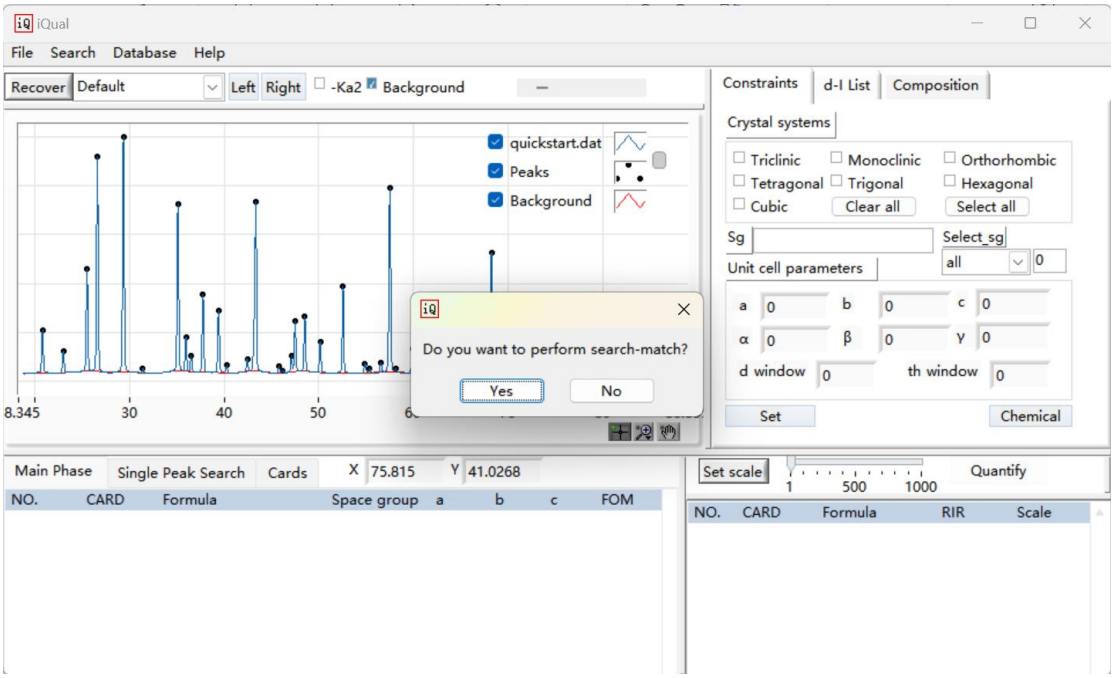
Graph menu:



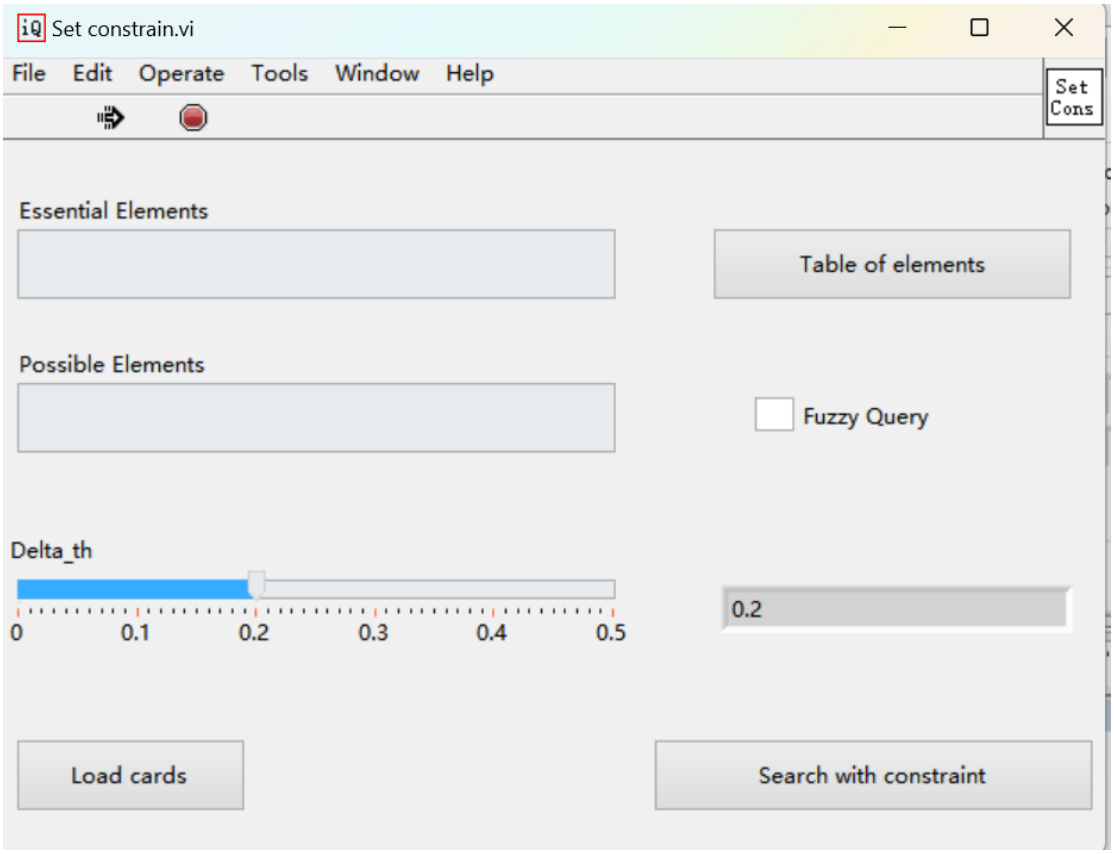
2. Choose a file to open it. Now it only support the CuKα's wavelength (1.5406), but we will add other wavelength later. We choose quickstart.dat as an example, which contains 56% Corundum, 22% Calcite and 22% SiO2 (Quartz).



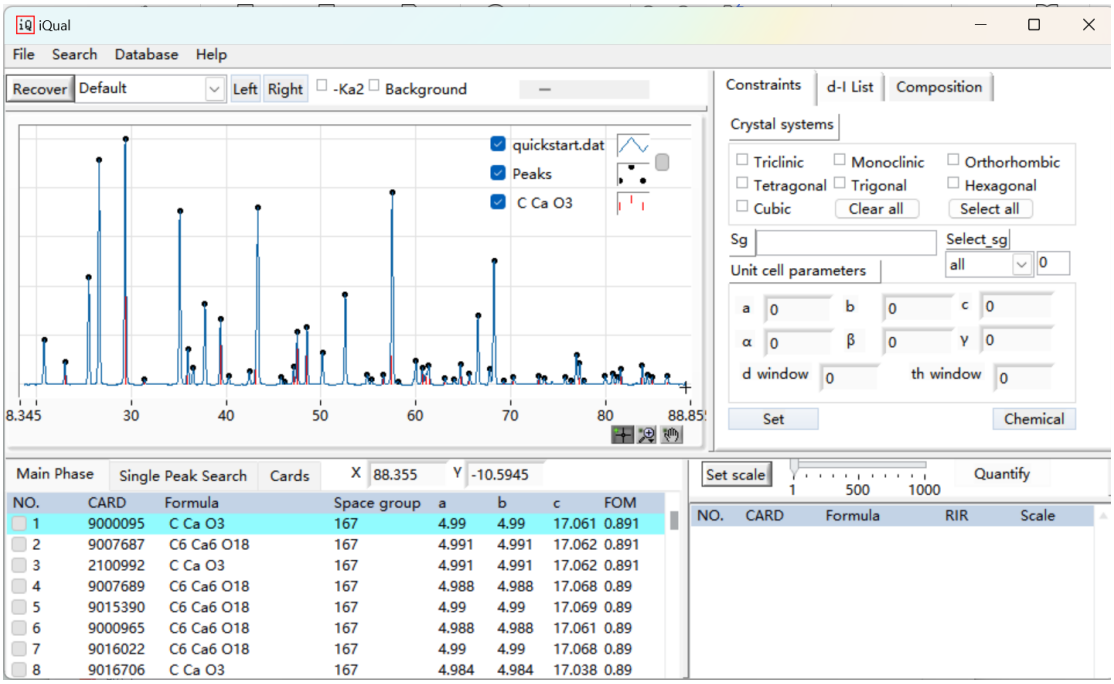
3. iQual will automatically find and subtract the background, and then detect peaks with default parameters (Threshold=10, Width = 8). You can perform search-match if you click “Yes”, or check the background or peaks (click “No”).

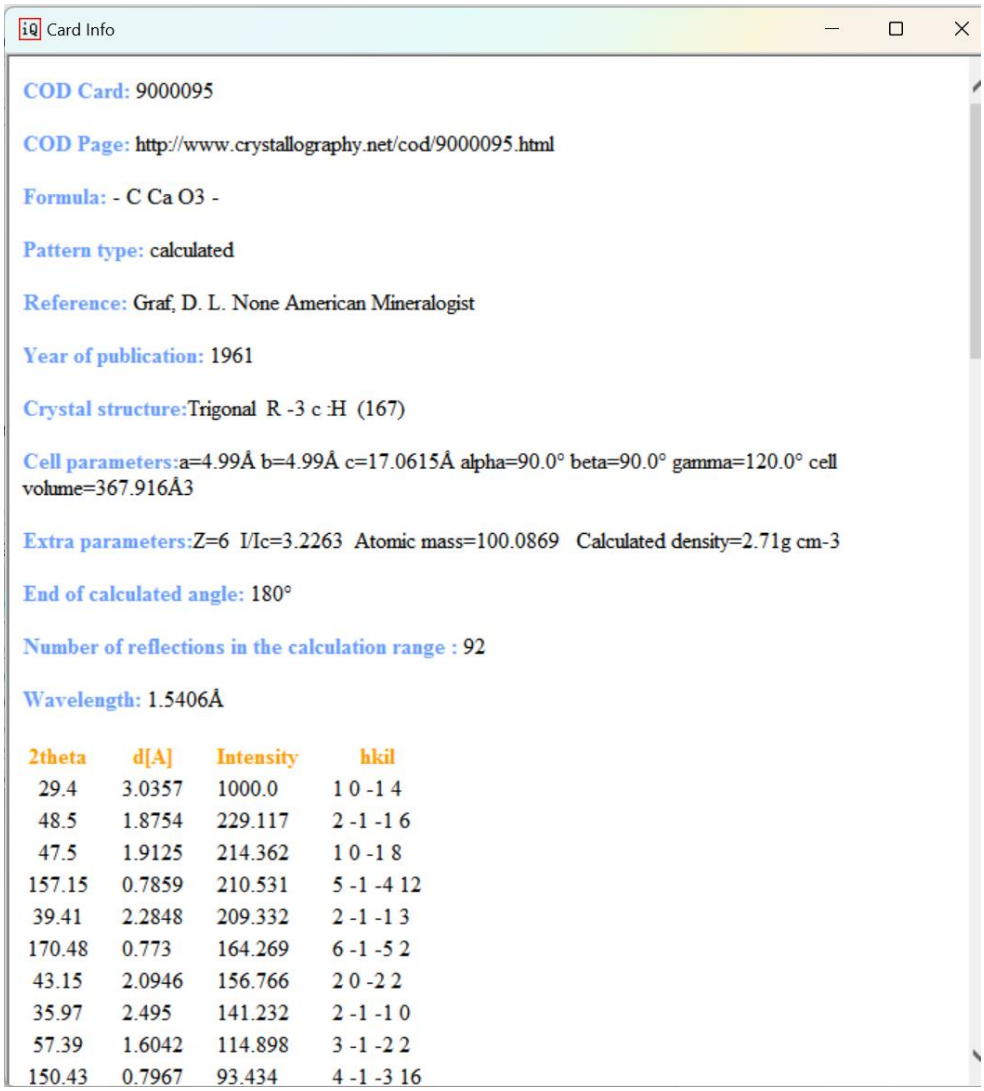


4. Usually you can click yes, and iQual will show the users the basic constraints including elements setting and theta window setting (If the differ between a peak from database and the experimental peak below “Delta_th”, it will be considered a matching peak)

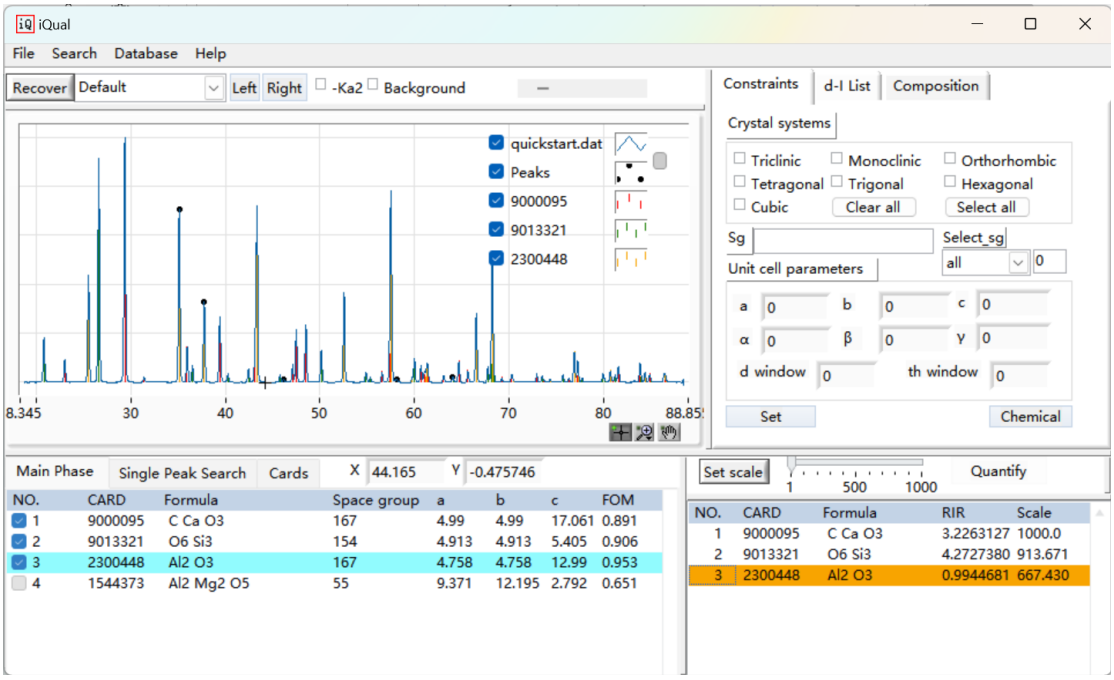


5. Then click the “Search with constraint”, iQual will perform a search-match by using the constraints, and return the candidate phases in the list. You can see the peaks of a candidate phase if you click it in the list. You can double click it to see the card of that phase.

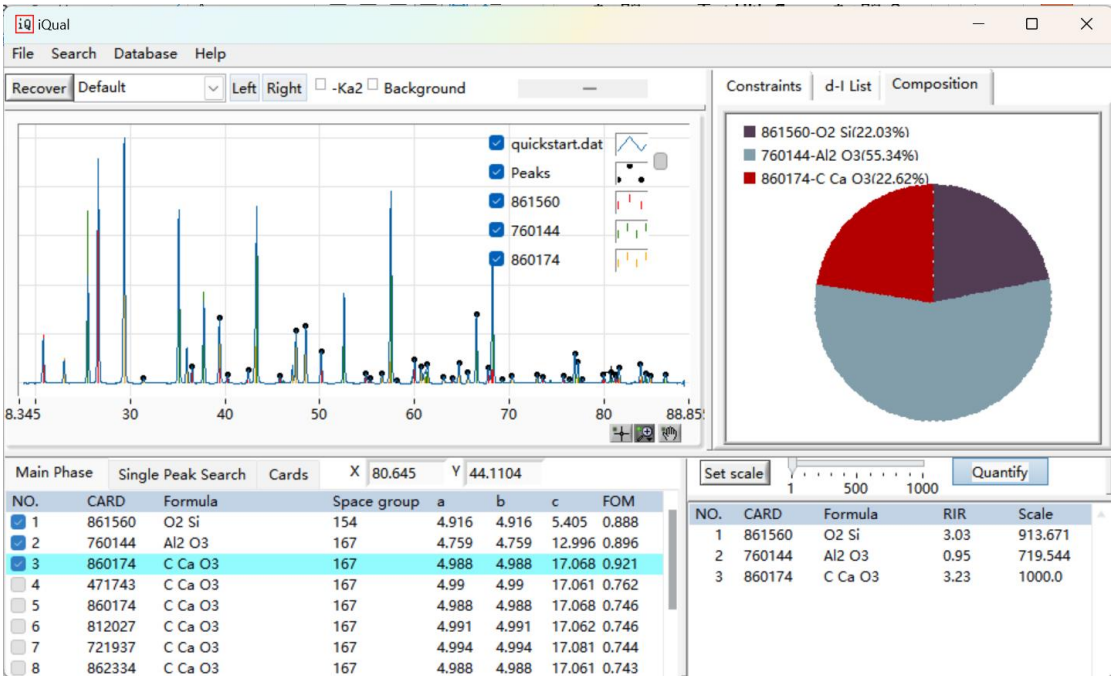




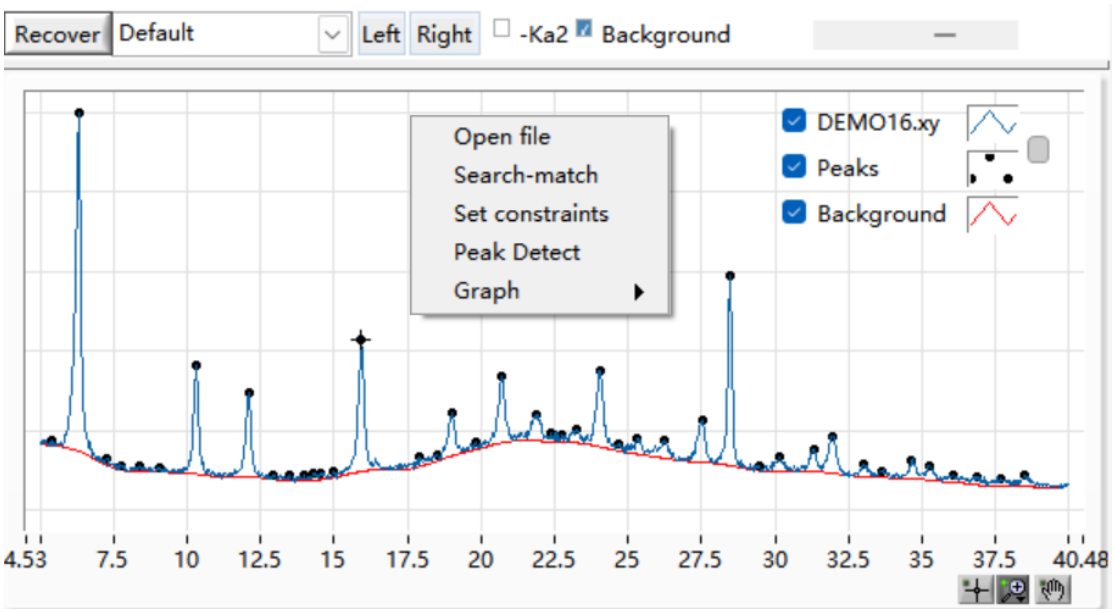
6. Select a phase by click the checkbox of that phase. If the user checks a candidate phase in the phase list, the experiment peak will be removed if the matched peak's intensity is more than 80% of the experiment peak's intensity, otherwise, it will be reduced by the matched peak's intensity. The remaining experiment peaks will be used for the next search-match if the user think it necessary.



7. You can click “Quantify” to perform a semi-quantitative analysis by using RIR (calculated I/Ic). Due to the RIR of PDF-2 comes from experiment, so we choose the PDF-2 database (parsed by iQual that has similar structure with Crystal_db). And the results which are 55.34%Corundum, 22.62% Calcite and 22.03% SiO2 (Quartz), which is very close to the true value of 56% Corundum, 22% Calcite and 22% SiO2 (Quartz).



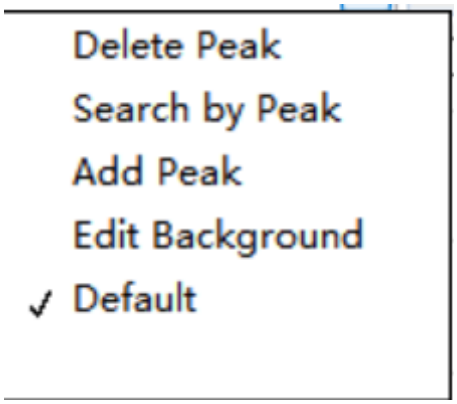
Graph operation



Operations to the graph can be done by using the components in the figure above.

: Use this button can set the graph into a suitable range.

: This dropdown box can be used to determine the response to the mouse. There are five options as the picture shows.



Delete Peak: Double click left mouse button to delete a peak if the cursor is near that peak.

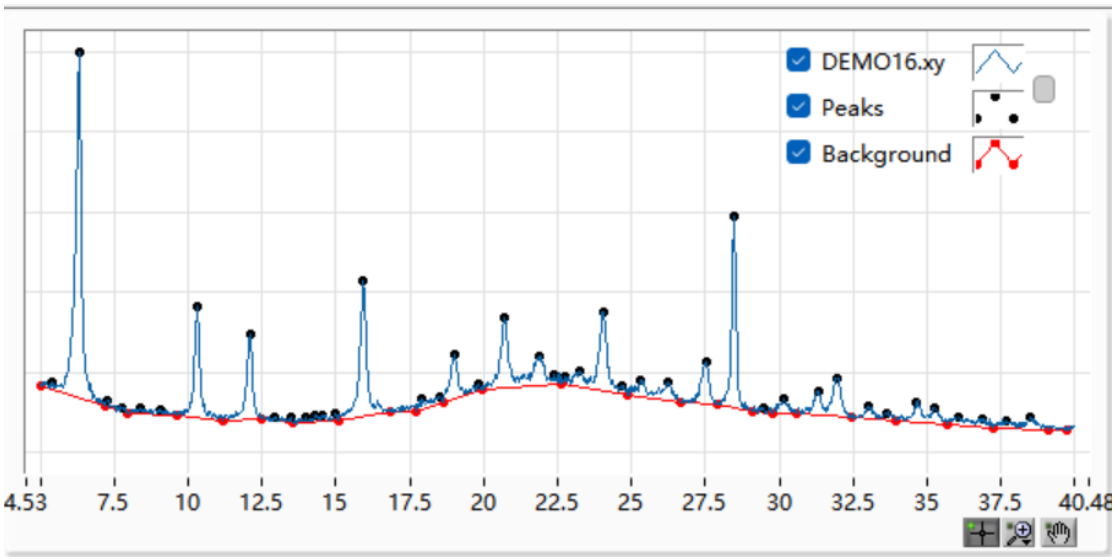
Add Peak: Double click left mouse button to add a peak at the position of the cursor.

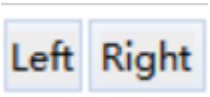
Search by peak: Double click left mouse button to perform a search-match using a

single peak.

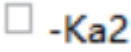
Edit Background: If user select this option, the program will show some valley points of the pattern, and linear interpolation of these points is used as the background. Then the mouse in the graph will turn to be a cursor, you can double click left mouse button to add a point and double click the middle mouse button to delete a point near the cursor. If you hold the left

mouse still over a point on the graph, you can move the point and it will be merged with other points near it.

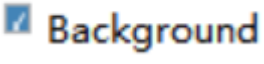




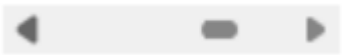
: These two buttons are used to aid the user to move the peaks of a select phase from database. Those features are used to check the zero shifts and we will improve this feature in the future.



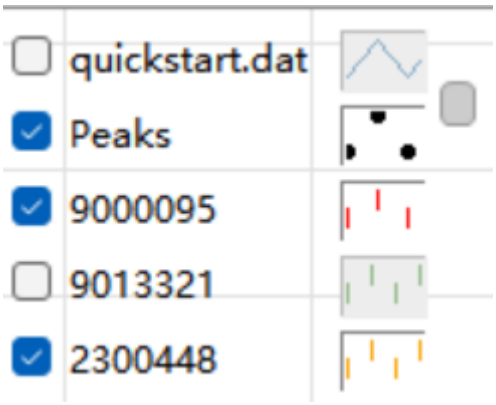
: This check box can help user to roughly remove CuKα2 peaks by using the wavelength and density relationships. We do not recommend this feature for mixtures and will improve this feature in the future.



: Show or hide the background.

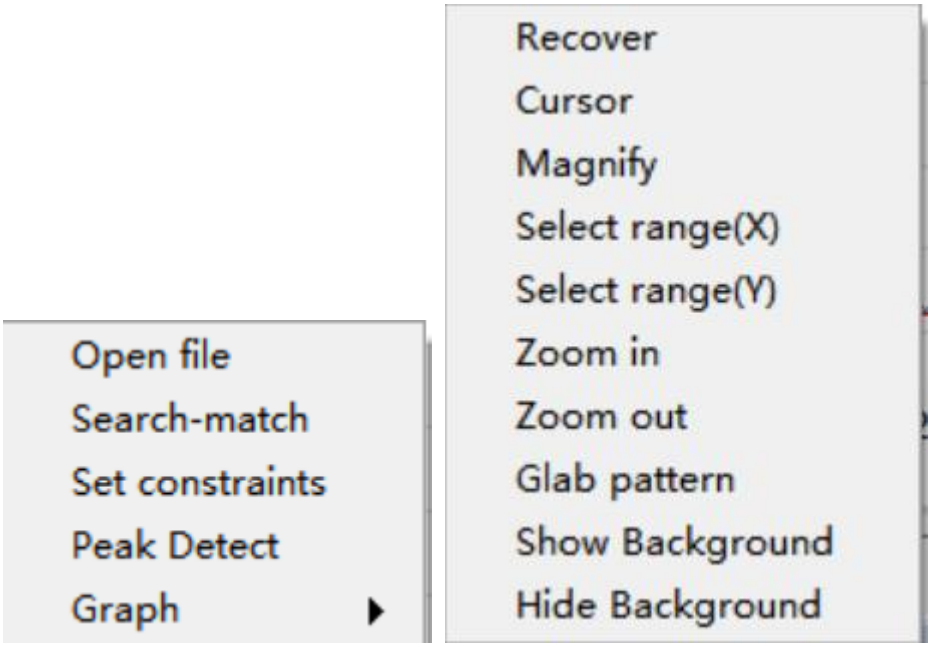

: This scrollbar can be used to move the graph.

Graph legend: Users can click the checkbox in the graph legend to let some graphs show or hide.



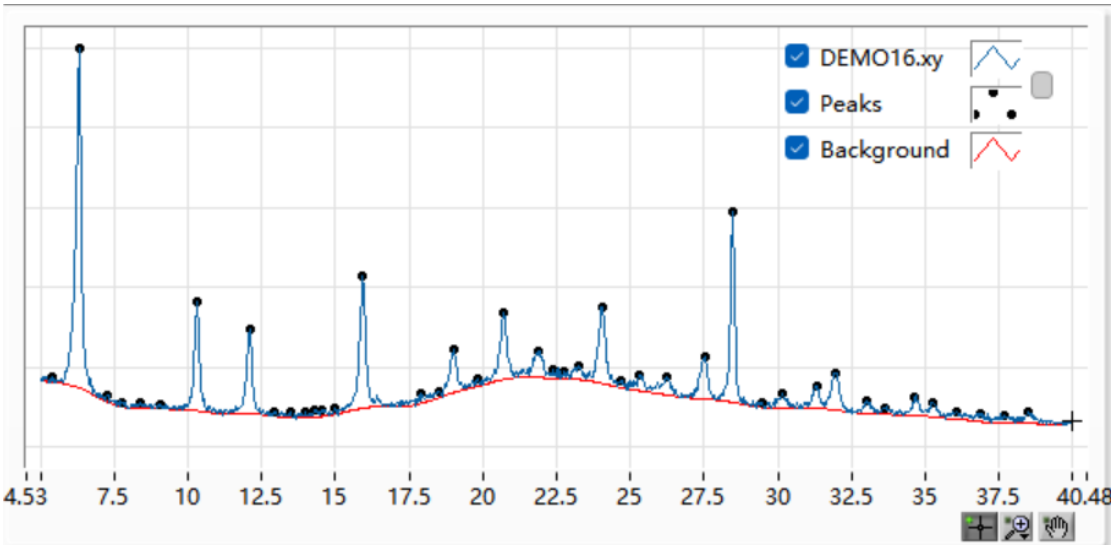
: Toolbar to operate the graph. The first one is the cursor, and will do nothing, but it you are doing the option like “Edit background”, you’d better use this. The second one and the third one can operate the graph, users can play to learn that.

Graph menu: Click right mouse button and you can see the graph menu. You can open file, search-match, set constraints, peak detect and choose graph operation by using it.

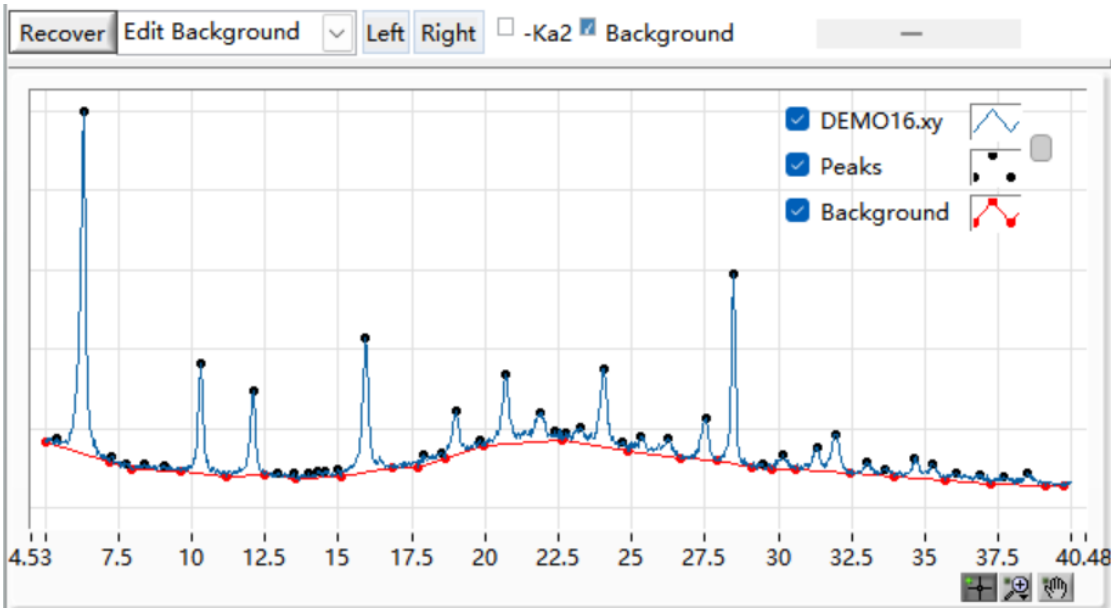


Background

The program uses Brückner algorithm by default to find background once the user open a file.



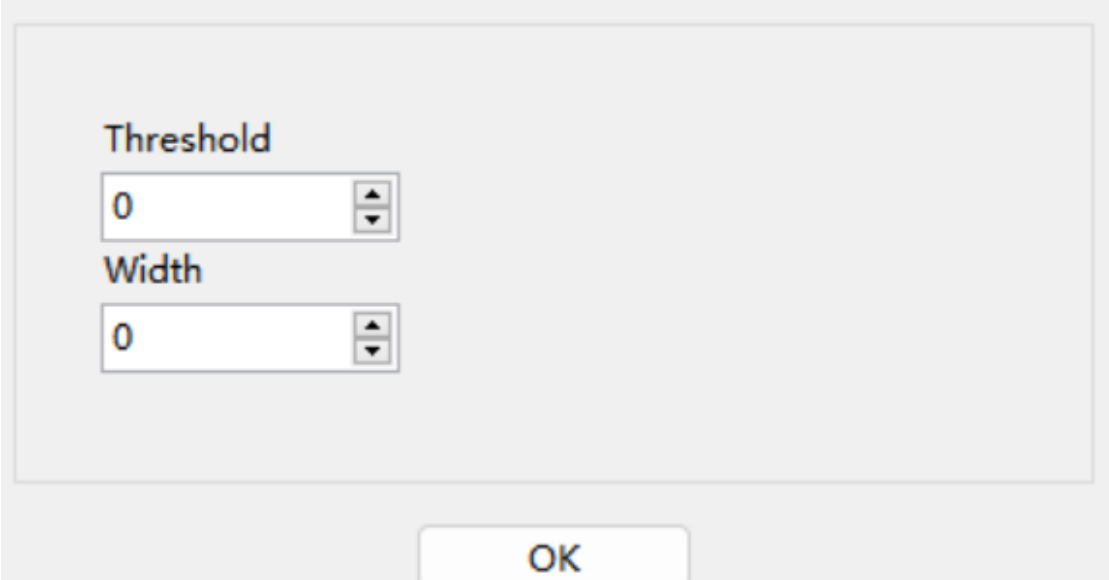
Users have the ability to edit the background points themselves. If the user chooses to “Edit Background", linear interpolation of these points is used as the background.



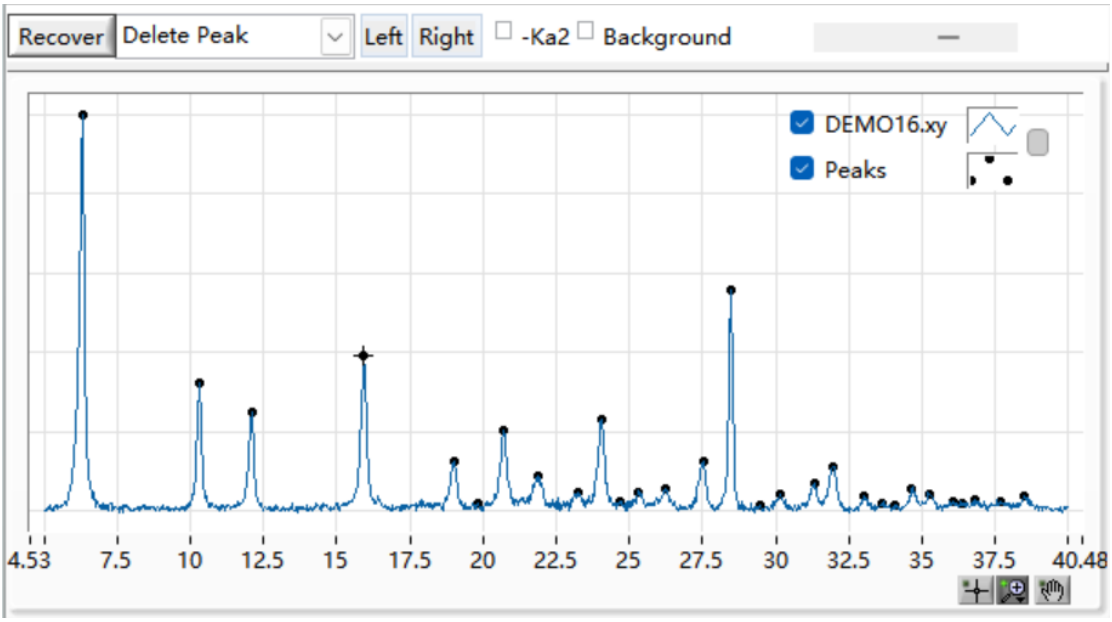
If user select this option, the program will show some valley points of the pattern, and linear interpolation of these points is used as the background. Then the mouse in the graph will turn to be a cursor, you can double click left mouse button to add a point and double click the middle mouse button to delete a point near the cursor. If you hold the left mouse still over a point on the graph, you can move the point and it will be merged with other points near it.

Peak detect

The peak search function is implemented using the tool library provided by Labview which uses the wavelet-based method. Users can set the intensity threshold and the peak width (number of points) to detect peaks, or they can add or delete peak in the graph. Usually, the intensity of the experimental pattern is automatically scaled to a maximum of 1000, so you can use 10 for example as the threshold. Width means the minimum number of points in the peak, usually you can set 8 and you can set a small number if there are some peaks are overlapping.

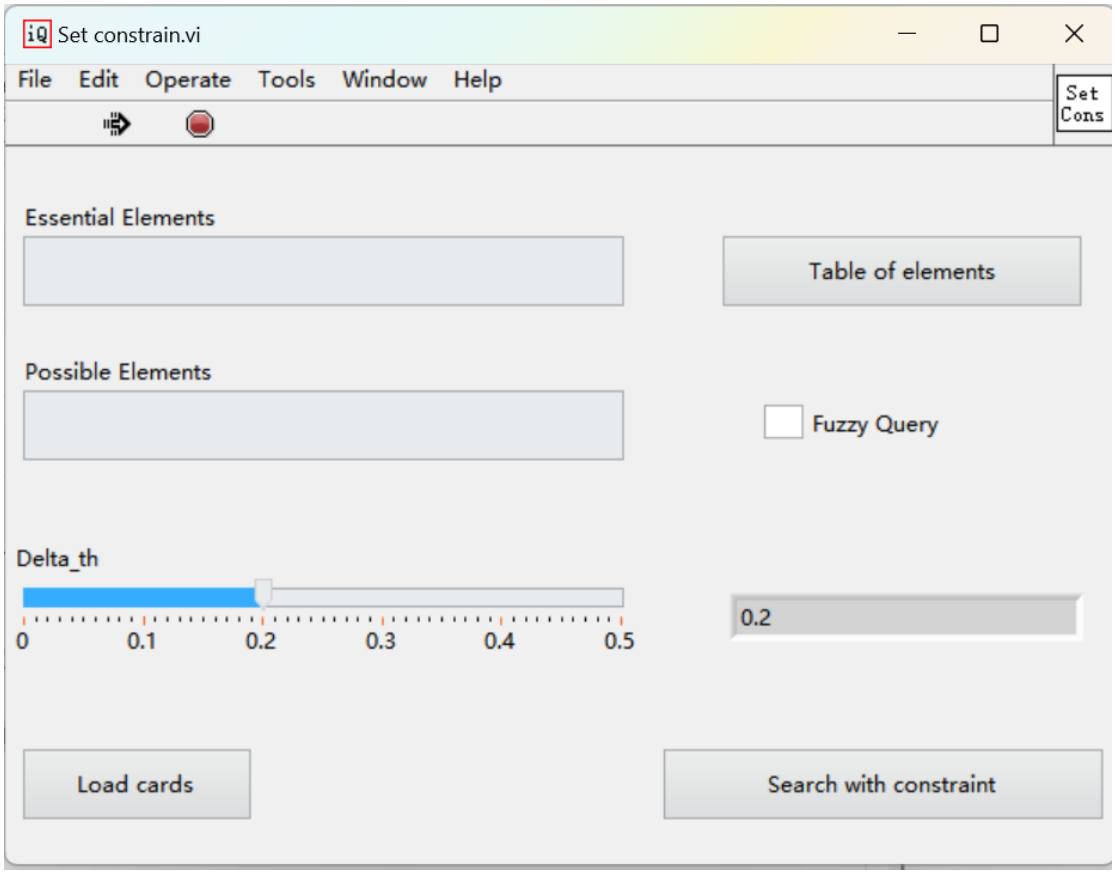


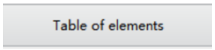
User can also add or delete in the graph by themselves. They can select the options in the dropdown box, and double click the left mouse button to do it.

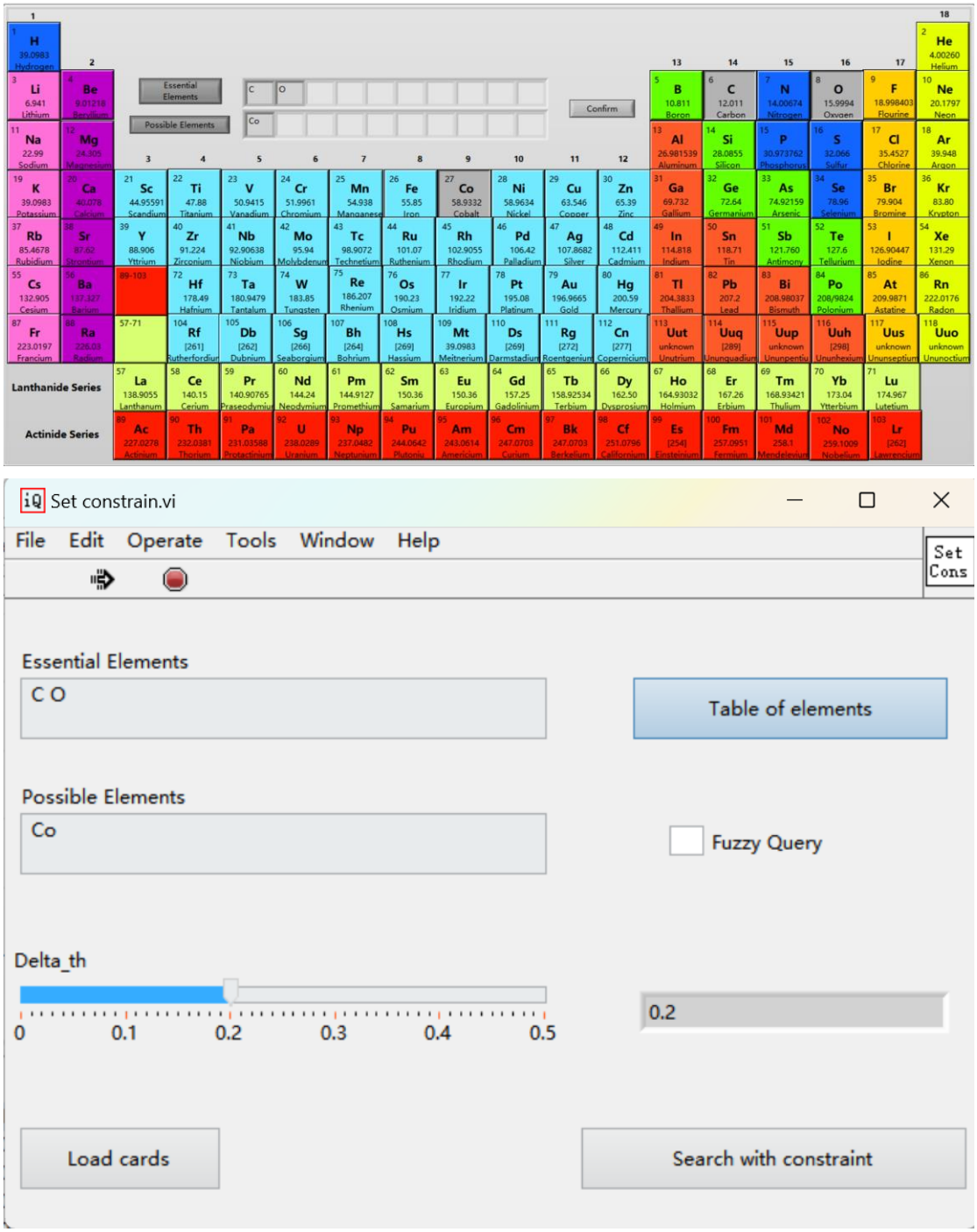


Set constraints

Basic constraints: The program will that window if you select “Set constraint” in both main menu and graph menu, or if you choose to search-match after the data file is open. The “Delta_th” means that if the absolute value of the difference between an experimental peak and a database peak is below it then these two peaks are considered to match each other.

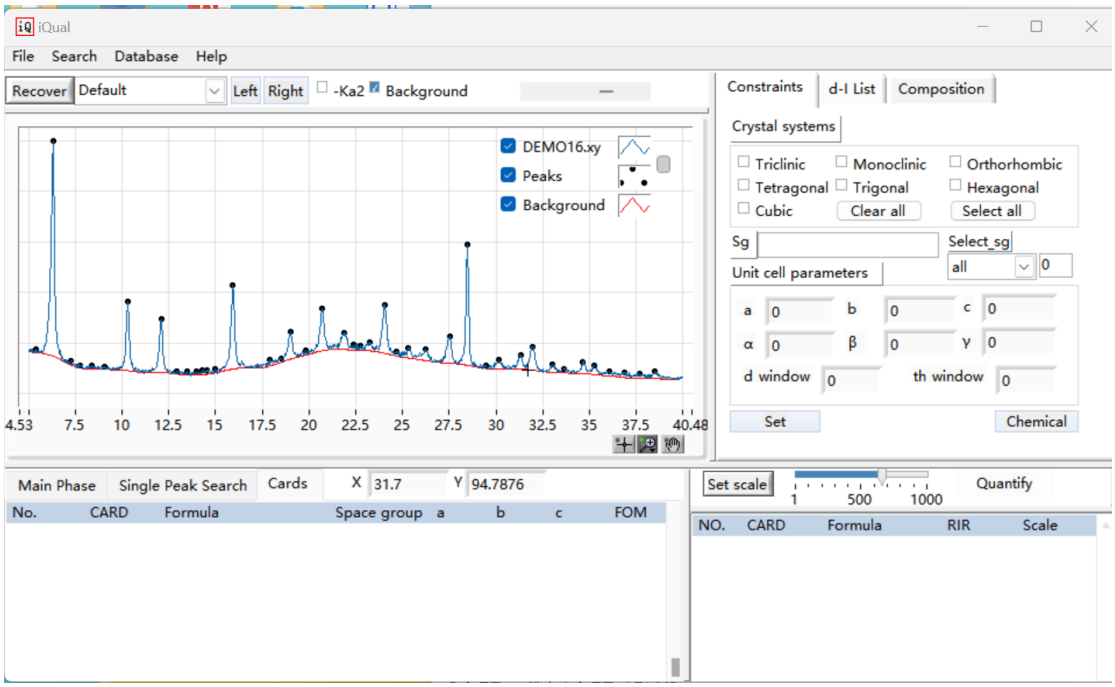


Users can click the  to choose element from the elements table. In the elements table, users can click the elements (its color will become gray), then decide they are essential elements (must be contained in the results) or possible elements (contain at least one), then click “Essential Elements” or “Possible Elements”, then the elements will in the lists. Users can finish this process by click “Confirm” button.



If the “Fuzzy Query” did not be select, the results will only contain the elements you have been selected, otherwise, it will contain other elements. Then users can choose to “Search with constraint” or “Load cards”.

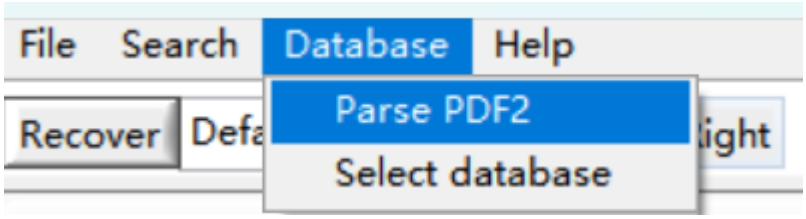
There are also other constrains such as crystal systems, space groups, cell parameters. The “d window” or “th window” means the range of the cell parameters, for example, if you set “alpha” = 90, “th window” = 0.5, then the results will be the phases with their alpha between 89.5 and 90.5.

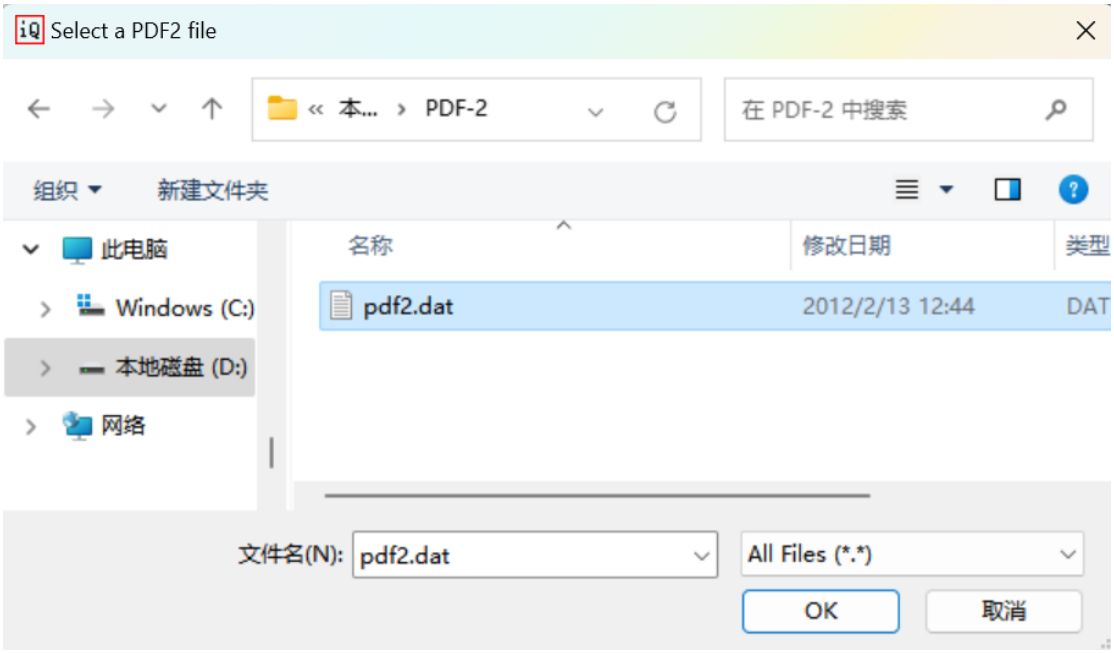


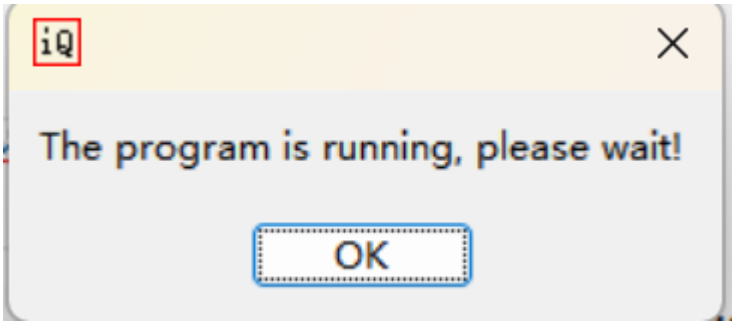
Database setting

Parse PDF2:

We provide the function of parse the PDF-2 database. Click “Parse PDF2” to choose a PDF-2 file, then the program will start to parse PDF-2 file and create a database that has the same structure with Crystal_db.

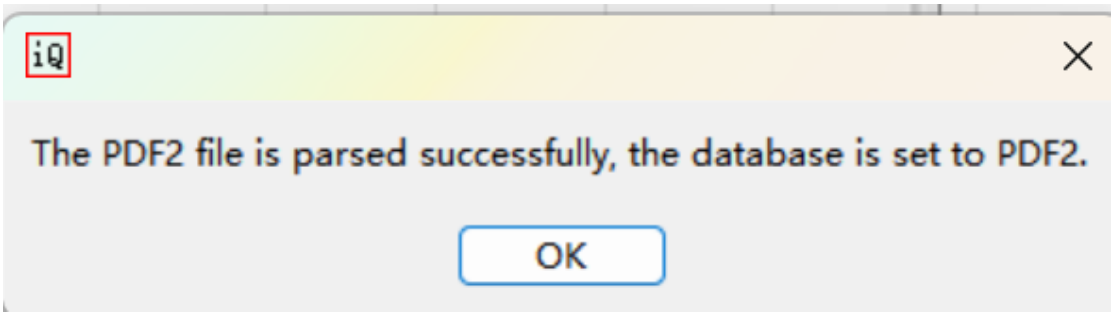




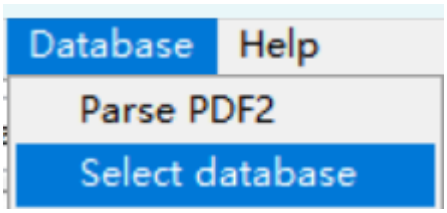


Click ok, and wait.

The program will tell you when it finished.



The user can also choose the database when the program is running (Crystal_db or PDF-2).



Search-match:

Users can click "Search-match" in both main menu and graph menu to perform a search-match using 3 strongest peaks in the peak list, which will search candidate phases and calculate their FOM. Be careful for that the search-match will be conducted using the constraints settings, so check the settings before search-match. The result will in the list. User can also choose "Search by peak" option, and double click left mouse button to perform a single peak search.

Calculation of FOM:

$$\mathrm{FOM} = \sqrt[2]{\frac{\mathrm{FOM}_{th} * \mathrm{W_{th}} + \mathrm{FOM_i} * \mathrm{W_i} + \mathrm{FOM_{ph}} * \mathrm{W_{ph}} + \mathrm{FOM_{db}} * \mathrm{W_{db}}}{\mathrm{W_{th}} + \mathrm{W_i} + \mathrm{W_{ph}} + \mathrm{W_{db}}}}$$

$\mathrm{W_{th}}, \mathrm{W_i}, \mathrm{W_{ph}}, \mathrm{W_{db}}$ are the weights of four parts of FOM ($\mathrm{FOM_{th}}, \mathrm{FOM_i}, \mathrm{FOM_{ph}}, \mathrm{FOM_{db}}$).

$$\mathrm{FOM_{th}} = 1 - \frac{\sum_i^N |th_i^{exp} - th_i^{db}|}{\Delta * N}$$

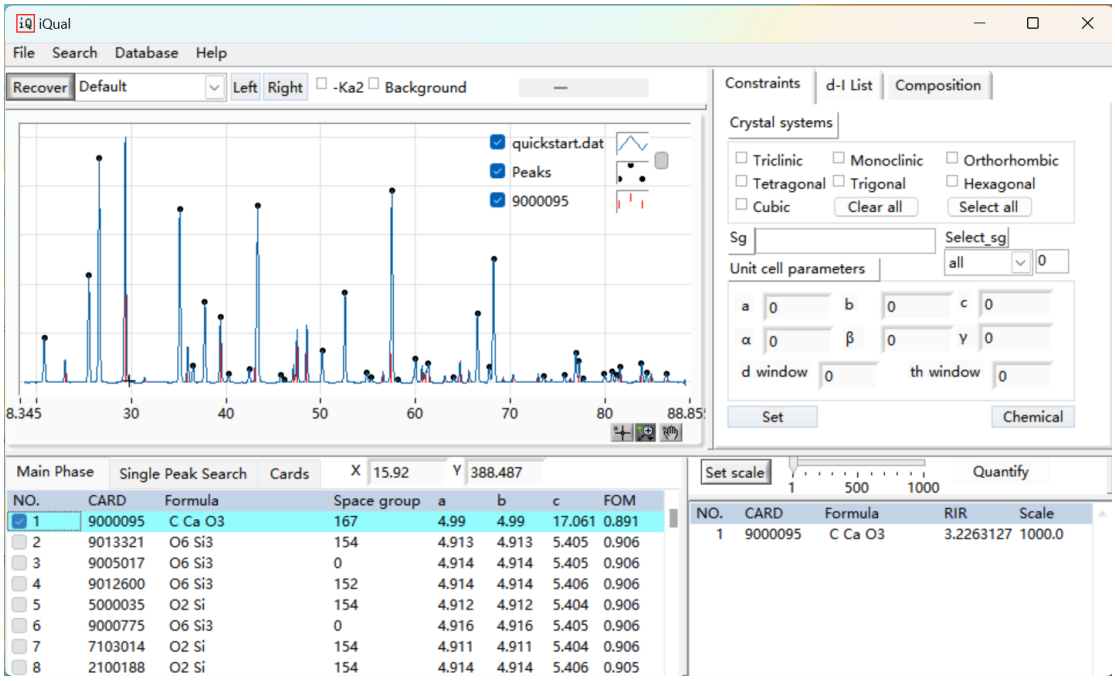
Δ is a user-defined theta window setting. If the absolute value of the difference between an experimental peak and a database peak is below Δ, then these two peaks are considered to match each other. N represents c matched experimental peaks, while $\mathrm{N_{db}}$ and $\mathrm{N_{exp}}$ represent the total number of the experimental peaks and the database peaks, respectively.

$$\mathrm{FOM_i} = \sum_i^N F\left(\frac{I_i^{db}}{I_i^{exp}}\right) * \frac{I_i^{db}}{\sum_j^{N_{db}} I_j^{db}}$$

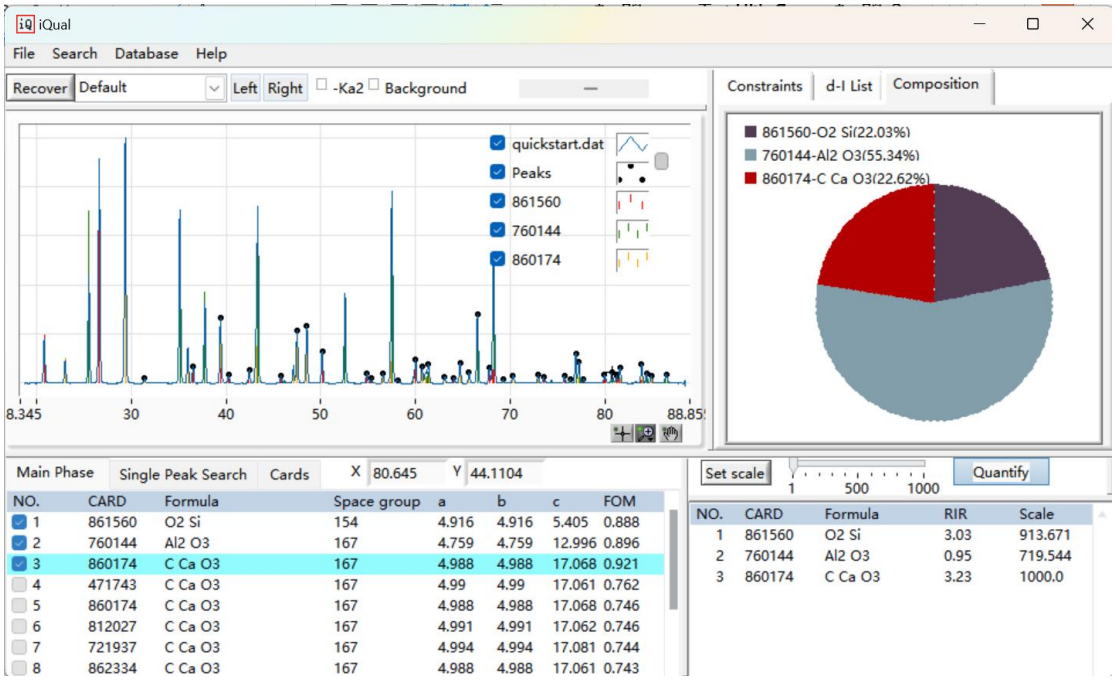
$$\text{Where } F(x) = \begin{cases} -1, & x > 3 \\ \frac{1}{2x}, & 1.5 < x \leq 30 \\ \frac{1}{x}, & 1 < x \leq 1.5 \\ x, & 0 < x \leq 1 \end{cases}$$

$$\mathrm{FOM_{db}} = \frac{1}{2}\left(\frac{\sum_i^N \mathrm{I_i^{db}}}{\sum_j^{N_{db}} \mathrm{I_j^{db}}} + \frac{\mathrm{N}}{\mathrm{N_{db}}}\right)$$

$$\mathrm{FOM_{ph}} = \frac{1}{2}\left(\frac{\sum_i^N \mathrm{I_i^{exp}}}{\sum_j^{N_{db}} \mathrm{I_j^{exp}}} + \frac{\mathrm{N}}{\mathrm{N_{exp}}}\right)$$



If the user checks a candidate phase in the phase list, the experiment peak will be removed if the matched peak's intensity is more than 80% of the experiment peak's intensity, otherwise, it will be reduced by the matched peak's intensity. The remaining experiment peaks will be used for the next search-match if the user think it necessary.

Semi- quantitative analysis

The program can use I/Ic to perform a semi- quantitative analysis. when the suitable phases have been selected, user can click “Quantify” to perform a semi- quantitative analysis. The scale uses the most-matched peak between experiment peak and database peak, user can also set the scale by select the phase in the phase list.