Welcome to TrueMatch

Welcome to the WITec True Match Database Search Software Help.

Installation	Infos about the installation
User Interface	Help for menu, spectrum selector, spectrum viewer, sample properties
Search	Help for all search features
Database Management	Handling custom databases and ST Japan integration

Press the **F1 key** anywhere in the software to open the
context help or browse the Help Menu to open the help contents

Installation

Installation

The WITec TrueMatch Software is delivered in a combined setup with WITec Project (or available as a separate .msi installer).
It contains the following software components:

- WITec TrueMatch Executable and all depending DLLs
- WITec ParticleScout and WITec TrueMatch are integrated in the same application

Program Start

TrueMatch is started automatically when exporting spectra from WITec Control or WITec Project to TrueMatch.
You can also start TrueMatch using the start menu of windows or the "WITec ParticleScout" shortcut on the desktop.

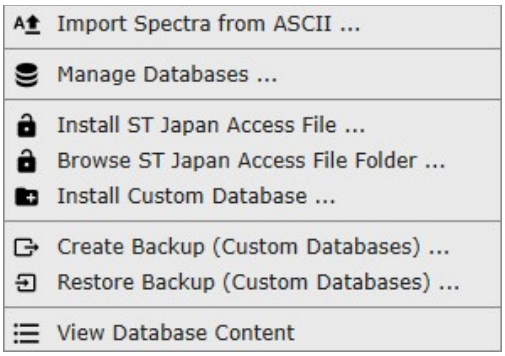
Licensing

A special TrueMatch license is needed to use TrueMatch without any limitations.
Once you have ordered the TrueMatch license, it is included in the WITec Project license and can be used on any number of computers.

Computer Requirements

- 4 Gb RAM minimum, 8 Gb recommended
- 1 Gb Hard Drive Space
- Direct3D compatible display adapter
- Windows 7 64-bit or Windows 10 64-bit
- .NET Runtime 4.7.1 or newer
  (Download Link: https://www.microsoft.com/net/download/dotnet-framework-runtime/net471)

TrueMatch Menu



Import Spectra from ASCII
This allows you to import spectra used for searching or to add into your own Database from an ASCII file.

Manage Databases
This opens the database manager. Here you can create or delete your own databases and show or hide the ST Japan and WITec Demo Databases.

Install ST Japan Access File
This will install the ST Japan Access File which is needed for running the ST Japan database. This file defines which ST Japan Sub-Databases are licensed. Also, a hardware USB Dongle must be used.
See ST Japan Database.

Browse ST Japan Access File Folder
Opens a explorer window and browses to the ST Japan Database folder.
See ST Japan Database.

Install Custom Database
Copies a .h5 database file into the TrueMatch custom databases folder.

Create Backup
This will put all your custom databases into a compressed ZIP file.

Restore Backup
This will restore custom databases from a compressed ZIP file. You will be asked if a database already exists.

View Database Content
This will open a database viewer which allows you to browse through all databases.

Spectrum Selector

Spectrum Selector

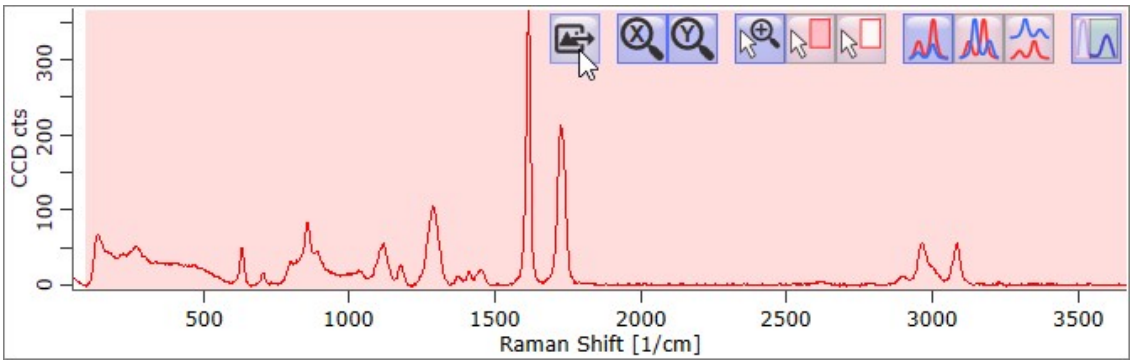
If multiple spectra are sent from WITec Project or were imported, you can select the current spectrum with the Spectrum Selector.
This will change the red preview graph to the selected spectrum and show the selected result.

If you want to add a single spectrum to a custom database, the currently selected spectrum will be added.

You can remove a spectrum from the list using the remove button on the right.

Spectrum Viewer

Spectrum Viewer



The Spectrum Viewer shows the user spectrum as a red graph and the selected result or database spectrum as a blue graph.
Right from the viewer there is a legend showing the names of the graphs.

Buttons (from left to right)

Export
This allows you to export the current view into a image file or to a preview where you can define the line width, font size etc.

Zoom X
Auto Zooms the X-Axis. Right-Click to turn on/off the automatic X-Axis Zoom on graph change.

Zoom Y
Auto Zooms the Y-Axis. Right-Click to turn on/off the automatic Y-Axis Zoom on graph change.

Mouse Zoom Mode
If selected, you can simply drag a region with the left mouse button to zoom that region.
Double-Click to automatically zoom the X- and Y-Axis.

Mouse Set Mask Mode
If selected, you can drag a region (drawn as red background) to set mask pixels.
This way you define which spectrum pixels should be used for the search or to add into the custom database.
Double-Click into the viewer to reset the region to the default region defined in the **Search Options**.

Mouse Clear Mask Mode
If selected, you can drag a region (drawn as red background) to clear mask pixels.

Same Y Axis
If selected, uses the same Y-Axis for all spectra.

Overlay Y Axes
If selected, each spectrum has its own Y-Axis and will be automatically zoomed to fit the window height.

Stacked Y Axes
If selected, each spectrum has its own Y-Axis and will be stacked above each other.

Options

Show X/Y Axis
Show or hide the X/Y Axis drawing.

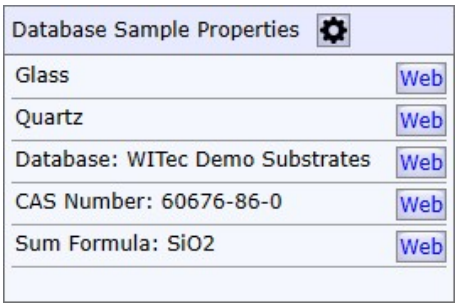
Hide Rayleigh Peak
If checked, the Rayleigh Peak will be hidden upon automatically zooming the X-Axis. You can zoom in and out the X-Axis any time using the mouse wheel (and holding the control key on the keyboard).

Zooming with the Mouse

You can simple turn the mouse wheel for zooming the Y-Axis.
Holding down the control key will zoom the X-Axis.
In the Mouse Zoom Mode, you can also drag a rectangle to zoom that region.
A double click into the viewer will zoom out automatically.

You can move the mouse to a position and press the <Space> key on the keyboard.
This will zoom into the region at the mouse cursor.

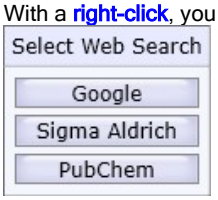
Sample Properties Display



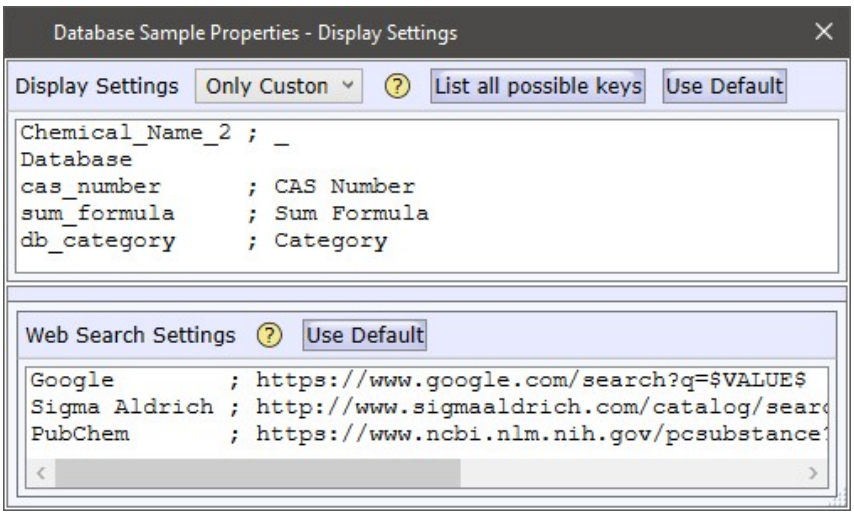
The Sample Properties box shows certain additional information about a database spectrum or search result.
For editing Sample Properties of your own custom database, see Database Editor and Sample Property Editor.

Web Web Search
You can click on the Web button in order to search for a certain property (uses default search).

With a right-click, you can select between a customizable list of searches:



Open Settings
You can define which properties should be displayed and also define a web link for each kind of information:



Display Settings

Show All (ComboBox)
You can select between the following options:

- Don't show: shows no properties
- Show All: shows all sample properties, no matter which are defined in the text. Though your definitions will be used.
- Only Custom: shows only the defined sample properties

List all possible keys
Enumerates all info keys from all databases and shows them.

Use Default
Uses a default set of sample properties.

Text Box
Here you can define, which properties should be shown.
Syntax:

<Property Name> ; <Optional Display Name>

Web Search Settings

Here you can define any number of web search URLs that can be used to search all sample properties in the web.
Each line in the text box defines a search.

The first line is the default search which is performed on a left click.

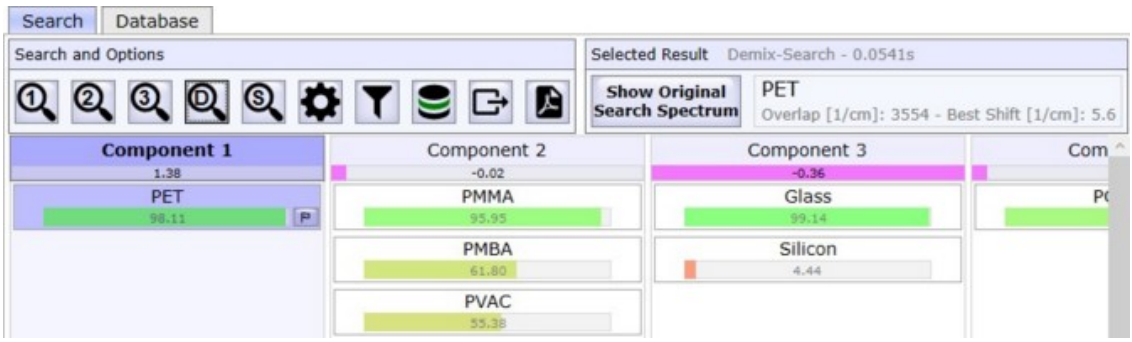
Syntax:
<Search Name> ; <Search URL>

The string $VALUE$ in the Search URL will be replaced by the particular sample information.

User Spectrum Properties

The small button on the far right will show the properties of the user spectrum, if any set.
Here you can also define which properties should be shown.

Search Overview



Search and Options

Simple Search
This will start a simple database search: each unknown spectrum will be compared with each database spectrum.
Only spectra from databases and categories of the Main Search Set defined in the Database Selection are used.

2-Component-Search
This will start a two component search: two database spectra are mixed to fit the unknown spectra.
Only spectra from databases and categories of the "Set for Component 2" defined in the Database Selection are used.

3-Component-Search
This will start a three component search: three database spectra are mixed to fit the unknown spectra.
Only spectra from databases and categories of the "Set for Component 3" defined in the Database Selection are used.

Demix-Search
This will start the demix search: all unknown spectra are demixed to fit the database spectrum.

Self-Search
Starts the self search: only all unknown spectra are compared with each other.
Can be used to see if there are similarities between your unknown spectra.

Search Options
See Search Options

 Result Display Settings
See Result Display Settings

 Database Selection
See Database Selection

 Export Results
See Result Export

 Report
See Generate PDF Report

Selected Result

Shows information about the selected result, such as the full name and the overlap (the overlapping region of the unknown search spectrum and the selected database spectrum)

Show Original Search Spectrum (Visible on Demix Search Result)
If not checked: the fitted / demixed spectrum is shown
If checked: the original search spectrum is shown

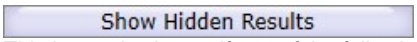
Arrow Buttons (Visible on Simple Search Result, if sorted by material)

Jumps to the result list of the previous / next material.

Result Lists

Shows the current search results.
For each unknown spectrum, one result list is displayed showing the best results on top.

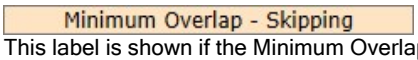
You can click any result with the mouse or move through the results using the arrow keys left/right/up/down.
You can select multiple results for exporting or for the report by clicking on the little flag or by pressing the space bar.



This button is shown, if one of the following settings lead to a result hiding:

- Minimum HQI
- Minimum Overlap
- Search/Filter Name
- Result deleted using the Delete-Key

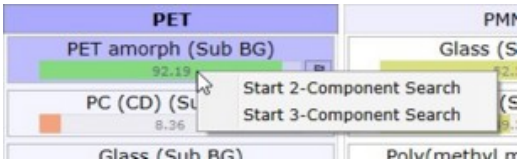
If this button is clicked, all results are shown again and deleted results are recovered.



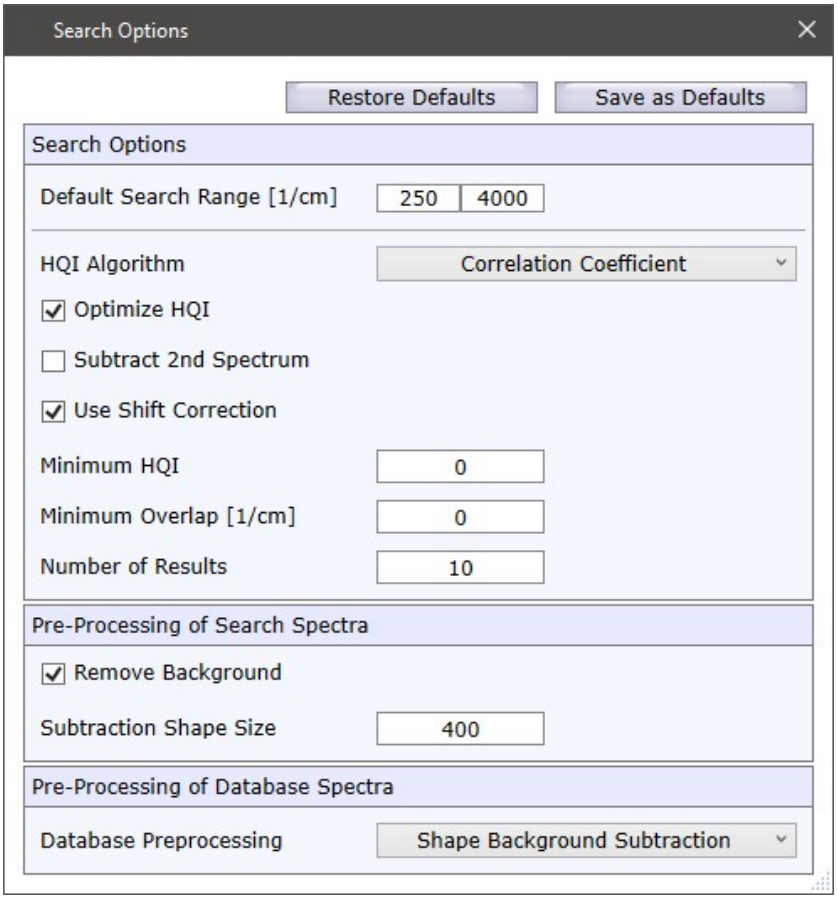
This label is shown if the Minimum Overlap in the Search Options leads to less results.

Use Result Database Spectrum for Multi-Component-Search

Right-Click on a search result in order to start a 2- or 3-Component Search using the result database spectrum as one of the components:



Search Options



Search Options

Default Search Range
Defines the default mask region for the search.
You can manipulate the mask in the graph viewer in order to define which part of the spectrum should be used for the database comparison.

HQI Algorithm
Defines the way how spectra are compared:

- Correlation Coefficient
- Absolute Difference
- Least Squares
- Euclidean Distance

See **Detection Algorithms**

Optimize HQI
Improves the HQI on noisy spectra.

Subtract 2nd Spectrum
Subtracts the 2nd Spectrum from the first one when using 2- or 3-Component Search.
E.g. subtract the substrate from the interesting material, thus reducing the influence of the substrate on the HQI.

Use Shift Correction
If checked, the search spectrum is shifted in a range of ±10 [1/cm] to get the best database match.
After searching, the shift with the best match is shown in the **Selected Result** area of the search tab.

Minimum HQI
Filters the result (only results with a minimum HQI are shown).

Minimum Overlap
Filters the result (only results with a minimum overlap are calculated and shown).

Number of Results
Defines the number of displayed results.

Pre-Processing of Search Spectra

Defines the preprocessing for the unknown spectra.

Remove Background
If checked, the background subtraction is done before searching. The WITec Project shape algorithm is used for the subtraction.

Subtraction Shape Size
Defines the shape size for the background subtraction. A lower value will subtract more details from peaks.

Pre-Processing of Database Spectra

Database Preprocessing
Defines the way how database spectra are preprocessed before comparing to the unknown spectra:

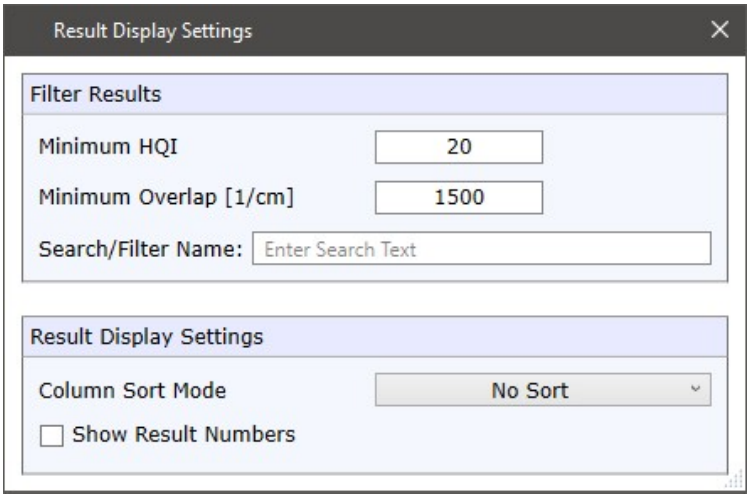
- No Preprocessing
- Use Derivative
- Shape Background Subtraction

Defaults

Restore Defaults
Uses the defaults and overwrites all current search options.

Save as Defaults
Saves the current settings as your defaults for future searches.

Result Display Settings



All display settings can be changed before AND after doing a search.

Minimum HQI
Filters the result (only results with a minimum HQI are shown).

Minimum Overlap
Filters the result (only results with a minimum overlap are shown).

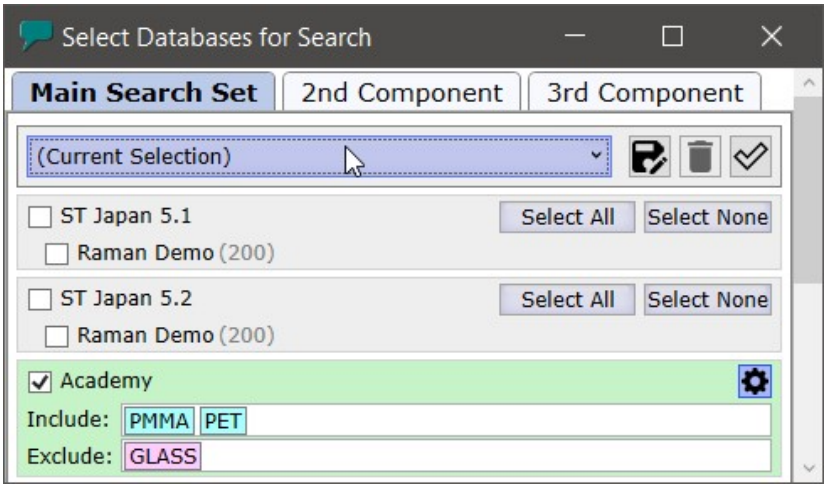
Search/Filter Name
Can be used to filter the result lists by database sample name.

Column Sort Mode

- No Sort - Uses the order of search spectra (imported or from WITec Project/Control)
- Best HQI - Sorts result columns by the HQI of the best result
- Material Name - Sorts result columns by the material name of the best result
- Best HQI & Material Name - Sorts result columns by the HQI of the best result and groups by the material name

Show Result Numbers
If checked, shows a result number / index on each result

Database Selection



Databases used for Search
Here you can select which databases should be used for the search.
The ST Japan contains multiple categories that can be checked or unchecked.
If no ST Japan Dongle and Access File is present, only the Raman Demo category containing 200 random Spectra is available for testing.

Main Search Set
This selection is used:
- for the simple search
- as the first component for a 2- or 3-component search
- and for the demix search

2nd component
This set is used as a second component for the 2- or 3-component search

3rd component
This set is used as a third component for the 3-component search

Current Selection (ComboBox)
When selecting a search set using the combo box, all selections are changed according to the saved selections.

Save current selection as new "Search Set"
Creates a new set from the current selection. You have to enter a name that will be used in the set selection combo boxes.

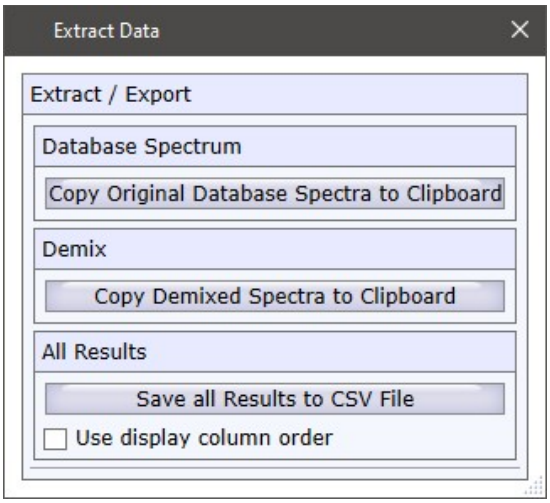
Delete selected
Deletes the selected main search set from your search set list.

Select All / None
Toggle select all or none of the databases.

Include / Exclude
Type a sample name you want to include or exclude in your search. Hit the Enter or Return Key to accept the sample name.
If names are included, only samples with the given names are used for the search.
If names are excluded, samples whose name matches the typed names will be excluded for the search.

Note: All sets and selections are stored on the hard drive.

Result Export



Copy Original Database Spectra to Clipboard
Copies the original database spectrum to the clipboard. Only works with custom databases.
When adding spectra to a custom database, the original spectrum is always stored additionally with the preprocessed search spectrum.
You can paste the data into any WITec Project instance.

Copy Demixed Spectra to Clipboard
Copies the demixed result spectrum to the clipboard.
You can paste the data into any WITec Project instance.

Save all Results to CSV File
Saves all displayed results into a semicolon-separated ASCII file.

Use display column order
If checked, the results of the csv file will have the same order like the currently displayed result lists (e.g. sorted by HQI).
Otherwise uses the original order of search spectra coming from WITec Project or the import file.

PDF Report

Use Header
Defines if a header is used in all pages.

Caption
Defines the caption in the header

Logo File Name

Defines the logo file name which is displayed in the right edge of the header

Show User Spectrum
You can define whether the unknown user spectrum is shown in as a graph.

Show Database Spectrum
You can define whether the found database spectrum is shown in as a graph.

Show Mix Part Spectra
When doing a 2- or 3-component search, all mix parts can be shown as single graphs.

Show Infos about the Search
If checked, a simple information about the used search is added at the beginning.

Show Hit List
If checked, shows a list of all results for each component.

Use Footer
Defines if a footer is used in all pages, showing a page number and e.g. a user name.

User Name
Here you can enter your name that will be displayed in the middle of the footer.

Sample Properties
Here you can define which sample properties should be shown for each result.
In the field <Key Name> you can enter multiple keys separated with semicolon.
All found properties for the given key names are displayed using the <Display String>.
If the property is not found, you can define a "not found string". Leave it empty to not display anything if the property is not found.

Detection Algorithms

Common Notations

$$S = \frac{1}{N}\sum_{i=0}^{N-1} S_i \qquad R = \frac{1}{N}\sum_{i=0}^{N-1} R_i$$

$\vec{R}$: *Reference Spectrum or Database Spectrum*
$\vec{S}$: *Spectrum*
R : *Average of Spectrum* $\vec{R}$
S : *Average of Spectrum* $\vec{S}$
N : *Number of Pixels in Spectrum*

Correlation Coefficient

$$HQI_{Cor} = \frac{\sum_{i=0}^{N-1}(S_i - S)(R_i - R)\left|\sum_{i=0}^{N-1}(S_i - S)(R_i - R)\right|}{\sum_{i=0}^{N-1}(S_i - S)^2 \sum_{i=0}^{N-1}(R_i - R)^2}$$

Absolute Difference

$$HQI_{Abs} = \left(1 - \frac{V}{D}\right) \cdot 100$$

$$V = \sum_{i=0}^{N-1} |S_i - R_i|$$

$$D = \sum_{i=0}^{N-1} |S_i|$$

Least Squares

$$HQI_{LS} = \left(1 - \frac{V}{D}\right) \cdot 100$$

$$V = \sum_{i=0}^{N-1} (S_i - R_i)^2$$

$$D = \sum_{i=0}^{N-1} (S_i)^2$$

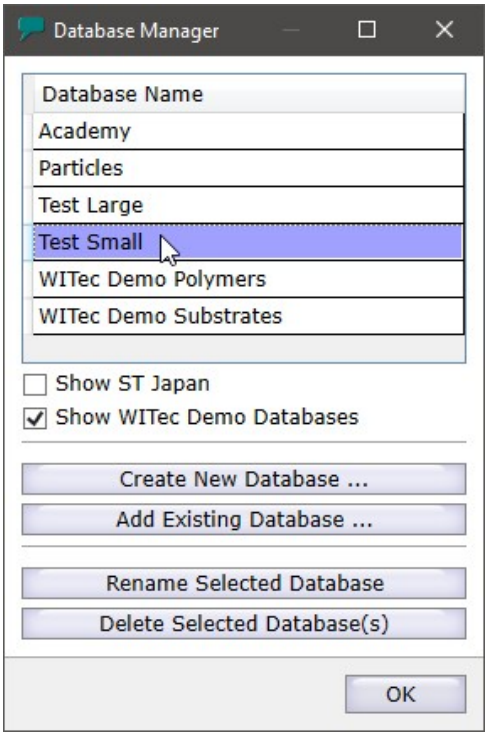
Euclidean Distance

$$HQI_{ED} = \left(1 - \frac{V}{D}\right) \cdot 100$$

$$V = \sqrt{\sum_{i=0}^{N-1} (S_i - R_i)^2}$$

$$D = \sqrt{\sum_{i=0}^{N-1} (S_i)^2}$$

Database Manager



The database list shows all databases that can be used for the search.

Show ST Japan
If checked, the ST Japan Database can be used for searching. If you don't have a dongle with accessfile, you can use the demo category of the ST Japan.
Uncheck if you didn't buy the ST Japan database.

Show WITec Demo Databases
Not yet supported: If checked, the WITec Demo Databases can be used for searching. Uncheck if you don't need those databases.

Create New Database
Creates a new customer database. The database file is automatically stored in a dedicated WITec databases directory.
You can backup and restore your databases using the TrueMatch Menu.

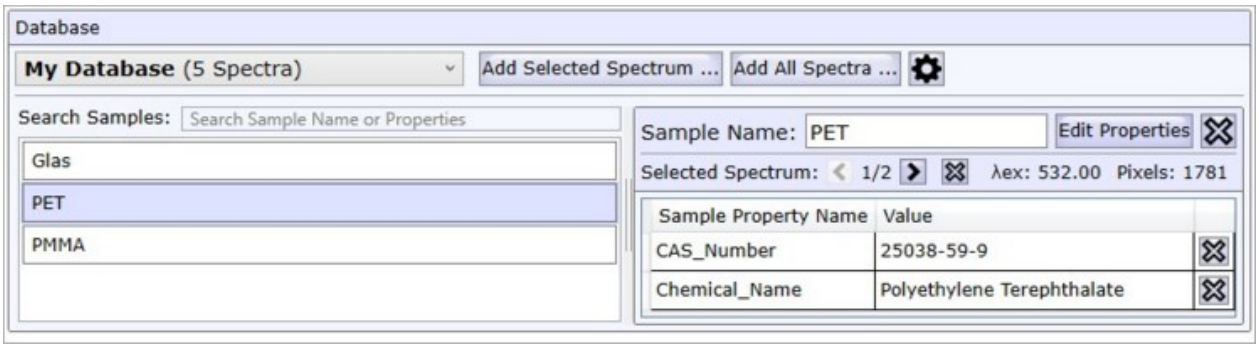
Add Existing Database

Here you can select a custom database file that will be installed in the dedicated WITec databases directory.

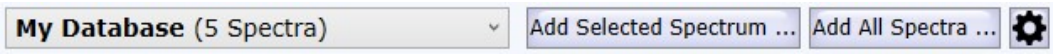
Rename Selected Database
Renames the selected database. The file name on the hard drive will be changed.

Delete Selected Database(s)
Deletes the selected customer databases from disk. The ST Japan and the WITec Demo Databases can not be deleted.

Database Editor



The Database Editor / Database Viewer can be used to browse all database spectra of all configured databases.
You can also add or remove samples/spectra to your own database.



"My Database" Database Selection (ComboBox)
Here you can select the desired database that you want to browse or to add spectra to.

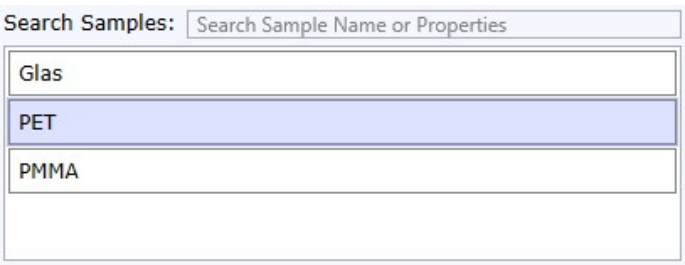
Add Selected Spectrum
Allows you to add the currently selected user spectrum to the selected database.
If a sample is selected, you can add the spectrum to this existing sample or you can create a new one (the software will ask you).

Add All Spectra
Adds all user spectra to the database and uses the names of each user spectrum as new sample names.
In WITec Project you can rename your single spectrum data objects, so the name is used here.

Add Options
See Add Options

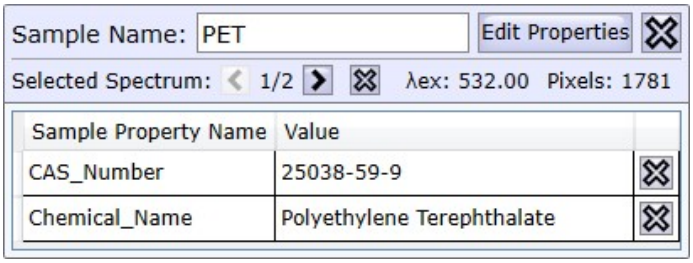
Current HQI

Shows the HQI of the selected user spectrum with the selected database spectrum.
Here you can also change the HQI Algorithm and create a report with those two spectra.



Search Samples
You can search in the sample names as well as in all sample properties.

Samples List View
Here you can select one of the samples. Clicking on a sample will show the first spectrum of the sample (there can be multiple spectra for each sample).
On the right side you can see details about the selected sample.



Sample Name
Here you can change the sample name, if a custom database is selected.

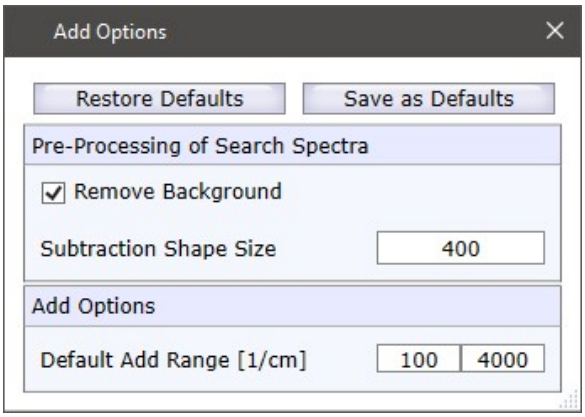
Edit Properties
You can edit the sample properties, see Sample Property Editor.

Selected Spectrum
If multiple spectra are stored for the same sample, you can browse through those spectra.
Some information about the selected spectrum are displayed: the excitation wavelength and number of pixels.

Sample Property List
Just shows all sample properties. You can delete properties here or by unselecting the "Use" Checkbox in the Sample Property Editor.

Add options

Here you can define which part of the spectrum should be added and also if the Rayleigh peak should be removed and a background subtraction should be done.



Remove Background
If checked, the background subtraction is done before searching. The WITec Project shape algorithm is used for the subtraction.

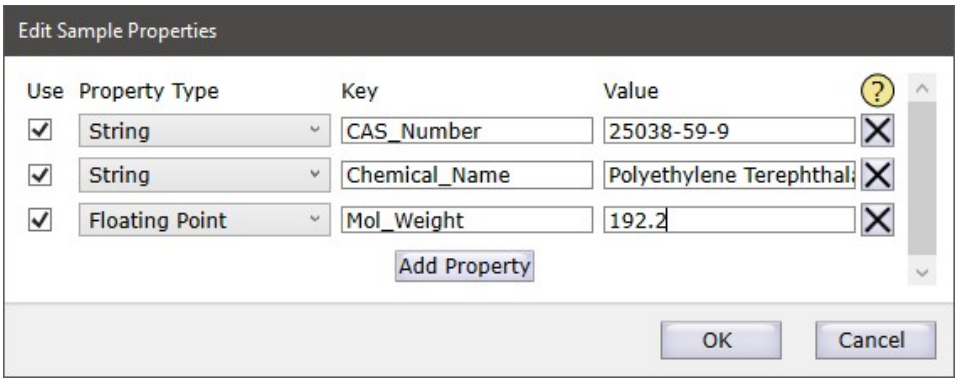
Subtraction Shape Size
Defines the shape size for the background subtraction. A lower value will subtract more details from peaks.

Default Add Range
Defines the default range that will be added into the database. You can manipulate the mask in the graph viewer in order to define which range of the spectrum should be saved as a database search spectrum.
Note: The original spectrum without preprocessing and region will be stored always in the database so you can reimport it to WITec Project after searching.

Save as Defaults
Saves the current Add Options as defaults.

Restore Defaults
Loads the defaults and overwrites the current settings.

Sample Property Editor



In the Sample Property Editor you can define your own property keys which are stored on the hard drive so you can reuse it for different samples/spectra that you add into your custom database.
The Property Type can be String, Floating Point or Integer.

To add properties to your sample, simply change the value of a property and the "Use"-Checkbox will automatically be checked (upon changing the keyboard focus to another edit or if you press enter).

ST Japan Database

Installation of ST Japan Database

The following installation files are available:

1. ST Japan (All Spectra), Version 51
2. ST Japan (All Spectra), Version 52 (newer with more spectra)
3. ST Japan Psychoactive, Version 52 (only psychoactive and drug substances)

The setup for 1 and 2 contains a demo license for 200 demo spectra.

Note that only WITec ST Japan Installation Files will work with TrueMatch / ParticleScout and you have to install the version which fits to your ST Japan License.

Installation of ST Japan License

After buying the ST Japan license, you will get an USB hardware dongle and a so called "Access File".
The Access File has the suffix ".stx".
To install the Access File, you can open WITec TrueMatch and then use the menu "TrueMatch -> Install ST Japan Access File".
Browse your Access File and click OK.
The software will ask you, whether you want to install the USB Dongle driver. If the dongle driver was not installed before, click yes.

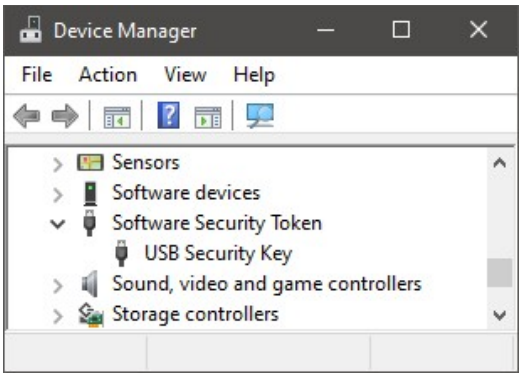
Make sure ST Japan is activated in the "Database -> Manage Databases .." Menu: "Show ST Japan".
Now the ST Japan license should work.

Before searching, you can define which databases and categories should be used for the search. Just click on this icon:


Troubleshooting

If the ST Japan is not working correctly, please consider the following solutions:

- Make sure the ST Japan USB Dongle is plugged in correctly.
- Ensure that the USB Hardware Slot is generally working.
- Check whether the USB Dongle is recognized by windows.
  For this, Open the device manager and look out for a "Software Security Token / USB Security Key"



If the device is not listed, ensure that the USB Dongle Driver is installed.
This normally happens automatically upon installing an Access file using the TrueMatch Menu.

- Make sure, the correct Version of the WITec ST Japan Database Setup is installed (51, 52, ...)
- Ensure that the correct .stx Access File is installed.
  In rare cases that you have installed multiple .stx Files (e.g. an older one which activates less spectra and a newer one which activates more spectra), you might have to remove the old/wrong .stx file using "Browse ST Japan Access File Folder" in the TrueMatch Menu.
- Make sure that the CheckBox "Show ST Japan" is checked in the Database Manager.
- Check whether the ST Japan Database or any of the available Categories is selected for searching.

ASCII Import

You can import one ore multiple spectra using the following ASCII format in order to execute a search or to add the spectra to a custom database.

The file must start with the [WITEC_TRUEMATCH_ASCII_HEADER].

Each spectrum must begin with the [SpectrumHeader] containing basic information about the spectrum.

Optionally, a [SampleMetaData] section can be defined in order to add some sample properties when adding the spectrum to a custom database.
The format is <key> = <value>, if "double" or "int" is preceding, you can define a floating point or an integer number as value.

At last, the [SpectrumData] data section must follow using one spectrum value per line,
beginning with the xdata / spectral position (in nm or 1/cm), followed by a <tabulator> character, followed by the ydata / CCD counts of this pixel.
The floating point number format must use a "." as decimal separator.

Example:

[WITEC_TRUEMATCH_ASCII_HEADER]

[SpectrumHeader]
Title = Component 1
ExcitationWavelength = 532.235
SpectrumSize = 1024
XDataKind = nm (or 1/cm)

[SampleMetaData]
CAS_NUMBER = 123-54578
double mol_weight = 63.123
int NumComponents = 2

[SpectrumData]
YourXData1 <tabulator> YourYData1
YourXData2 <tabulator> YourYData2
....
YourXData1024 <tabulator> YourYData1024

[SpectrumHeader]
Title = Component 2
ExcitationWavelength = 785.122
SpectrumSize = 1600
XDataKind = 1/cm

[SampleMetaData]
CAS_NUMBER = 123-11222
double mol_weight = 11.55

[SpectrumData]

YourXData1 <tabulator> YourYData1
YourXData2 <tabulator> YourYData2
....
YourXData1600 <tabulator> YourYData1600

...
...
...

Shared XData

For huge amount of spectra that share the same X-Axis values / XData, it is also possible to define the XData only once before the first [SpectrumHeader] is defined. This way, the ASCII save/load time can be reduced. In this case each spectrum only has to define the YData. The number of XData values must be the SpectrumSize and all spectra must have the same size.
Example:

[WITEC_TRUEMATCH_ASCII_HEADER]

[XData]
YourXData1
YourXData2
...
YourXData1600

[SpectrumHeader]
...
SpectrumSize = 1600
...
...