

HyperLab 2021

Reference Guide



HyperLabs Software

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About this document

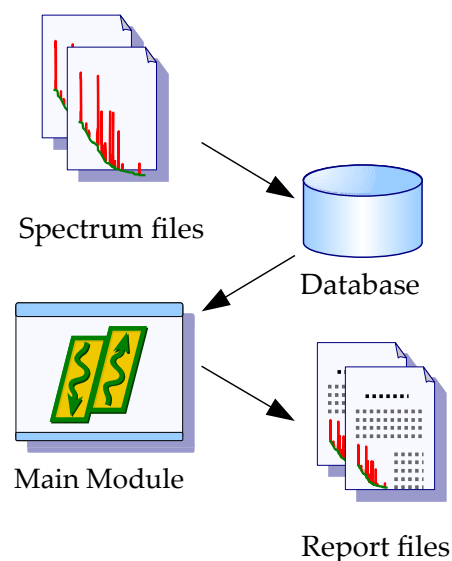
Start reading this *Reference Guide* for detailed description of HyperLab processes. For a short overview, refer *Quick Start Guides*, or read the *Installation Guide* if you are to install the system onto your computer.

1. System architecture overview

Databases are a well-developed technique in the business world, and HyperLabs Software strongly believes that it is the time to bring its power to the field of gamma spectroscopy. Therefore HyperLab Main Module stores *all* spectroscopic information in relational databases. The next figure illustrates basic system components.

Main module is the application where you will operate various evaluation utilities (peak area evaluator, detector efficiency evaluator etc.) and also the primary interface to information stored in one or more **databases**.

This Installation Guide describes two possible setup types: one is necessary to setup **HyperLab Main Module** application, the other is to install **Spectrum File Batch Evaluator** utility onto your computer. Batch Evaluator Utility does not require any database component to be installed, but therefore lacks features compared to the Main Module.



1.1. Benefits of database usage

Databases provide significant benefits compared to the conventional gamma spectroscopy, where a multitude of files are in use even if your system is of medium size.

Structured information storage

All of your data, including spectra, calibrations, peak evaluations, efficiency evaluation, etc. are stored in central locations grouped into user projects. Thus a highly integrated and structured set of information can be utilized. If you regularly backup *one single* database file, no measurement or evaluation data may be lost anymore.

No duplicated data

If you are using independent spectrum files, it is tempting to save all relevant spectroscopic information – e.g. detector efficiency data - into each spectrum file, to ensure that this information is not lost. If spectroscopic data is stored in databases, only a reference is required, which points from multiple spectra to a single detector efficiency curve.

Better integrity

Databases utilize strict integrity rules in order to prevent accidental data deletion. If a user wants to delete a measurement, it is possible only if no peak evaluation points to that data entry.

Easier post processing

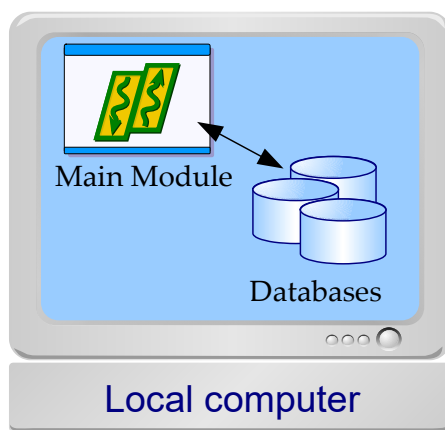
Databases provide the users with excellent resources and standard tool for post-processing: extraction of evaluation data is straightforward into e.g. spreadsheet applications.

1.2. Database topologies for Main Module

As HyperLab Main Module accesses data stored in HyperLab databases, and these databases may reside either on the local machine or on a remote computer, virtually unlimited number of database topologies may exist. The most common cases are detailed below.

1.2.1. Local database

The most common case is “Local database” topology, because only one computer is required in this arrangement.



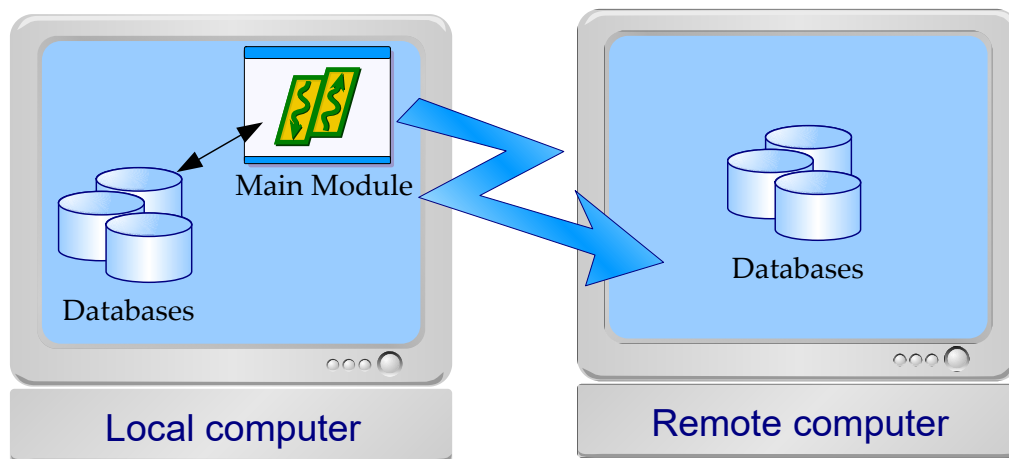
All HyperLab components must be installed on this sole machine, which will contain a local database management server software, as well as one or more local databases. Spectrum files have to be imported into the database, then the measurement entries are evaluated by the Peak Evaluator. The resulting peak entries are also stored back in the database. In this local database scenario, database access is performed at maximum speed, because network communication overhead is omitted.

Installation instructions

- Install all HyperLab components on the computer, including the Main Module and the Microsoft SQL database server.
- Create a local database from the Main Module: click on “Local Database Server” node, then select task “Create database” from the right and follow the instructions.
- Register the newly created local database in Main Module: click on “HyperLab databases” node, then select task “Register a local database” from the right and follow the instructions.
- Start using your newly registered local database.

1.2.2. Local and remote databases

It is always possible to use additional remote HyperLab databases on other computers in your local network – provided the remote database server allows incoming connections and you have the proper password assigned to those databases.



Advantages of remote databases

- Remote databases may be shared between working group members
- Database files and the SQL database server itself may be hosted on a powerful server computer, where regular backup is performed, so the chance for data loss is minimized.

Drawbacks of remote databases

- HyperLab disallows specific operations (e.g. database creation) on remote databases. In order to create a HyperLab database, you should run database creation utility on the destination machine.
- The networked database connection may be slower than accessing local databases.

Installation on the remote computer

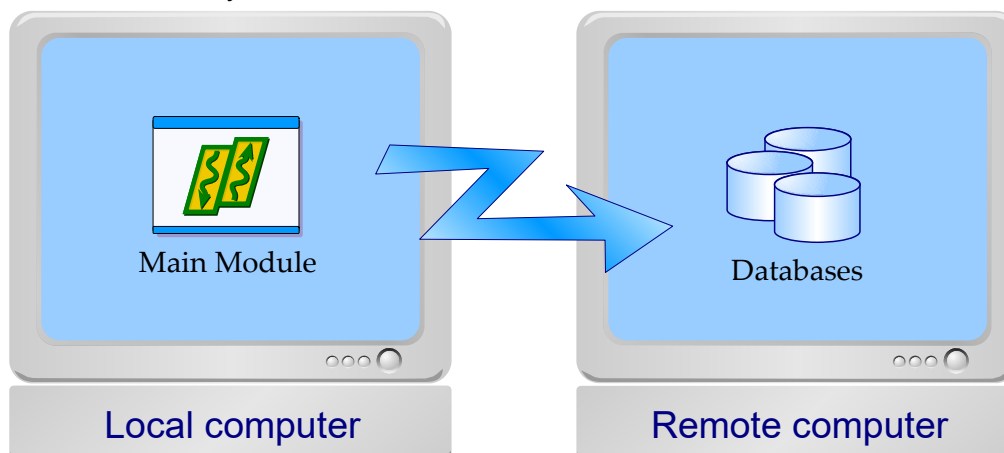
- Install all HyperLab components, including the Main Module and the SQL database server.
- Create a new database from the Main Module: click on “Local Database Server” node, then select task “Create database” from the right and follow the instructions.
- Make sure if the database server accepts incoming connections: click on “HyperLab databases” node, then select task “Manage database server” from the right. The management window appears now. Make sure that “TCP/IP” protocol is enabled. See “Configuring remote access” for further details.

Installation on the local computer

- Install all HyperLab components, including the Main Module and the SQL database server.
- Create a local database from the Main Module: click on “Local Database Server” node, then select task “Create database” from the right.
- Register the new local database in Main Module: click on “HyperLab databases” node, then select task “Register a local database” from the right.
- Register the remote database on the remote computer: click on “HyperLab databases” node, then select task “Register a remote database” from the right and follow the instructions. Specify the remote computer name as the database server host name.
- Start using your newly registered local and remote databases. Please note that the user name and password is tied to the database server – thus it is possible that you should specify different passwords for the local and the remote databases.

1.2.3. Remote database

This “remote database only” scenario is for advanced users.



It requires at least two computers on the local network: one contains the database server, while other processing workstation(s) only contains HyperLab Main Module, which accesses the remote databases through local computer network. This setup is ideal for working groups, where the database is installed on a central server, and a regular backup preserves the common database. The setup steps required for the two computer case are detailed below.

Installation on the remote computer

- Install all HyperLab components, including the Main Module and the SQL database server.
- Create a new database from the Main Module: click on “Local Database Server” node, then select task “Create database” from the right and follow the instructions.
- Make sure if the database server accepts incoming connections: click on “HyperLab databases” node, then select task “Manage database server” from the right. The management window appears now. Make sure that “TCP/IP” protocol is enabled. See “Configuring remote access” for further details.

Installation on the local computer

- Install HyperLab components without the SQL database server.
- Register the remote database(s) previously created on remote computer(s): click on “HyperLab databases” node, then select task “Register a remote database” from the right and follow the instructions. Specify the remote computer name as the database server host name.
- Start using your newly registered remote databases. Please note that the user name and password is tied to the database server – thus it is possible that you should specify different passwords for different remote databases.

2. HyperLab Main Module

Core of the HyperLab Gamma Spectroscopy System's visually rich evaluation environment is the Main Module. This provides simultaneous connections to multiple HyperLab databases, and makes it possible to interact with HyperLab objects which are stored in these databases.

You can start the Main Module by clicking on your HyperLab icon on the Desktop, or in your Start menu.

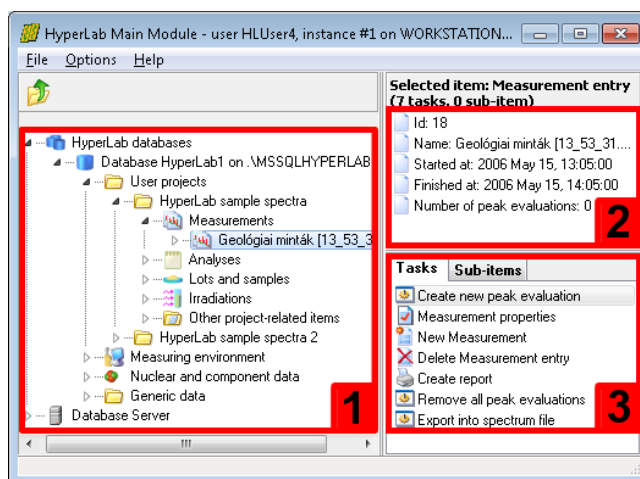
2.1. Main Module window

The most important parts of the Main Module's working window are the following:

Database browser tree [1] provides hierarchic listing of objects stored in HyperLab databases. The items displayed in this tree are called *nodes*.

Detail lister [2] shows common details for the item which is currently selected in the browser tree.

Tasks and Sub-items panels [3] also refresh their content according to the data entry you have selected in the database browser tree. *Tasks* provides you operations which may be performed on the selected database entry; whereas *Sub-items* shows special sub-components about it.



Content of the *Tasks* window also appears in a **context menu**, when the user right-clicks on a database node. Common **keyboard shortcuts** may help your work: the database tree may be walked through by using the *cursor arrow* keys, while the currently selected task may be started by hitting the *Enter* key. *Tab* key switches between the browser tree and the *Tasks* window.

2.2. Record editor pages

Record editors make it possible to enter details of a new database record, or modify the value of an existing entry. These data editing pages may be accessible if you select a data node in the database browser tree, and click on its property editing task.

Main features

Record editors support the following common operations:

- Field editing controls are grouped into pages under tabs.
- Non-editable fields are displayed as static (grayed) text.
- Field data may be entered into text boxes or are selectable from combo boxes.
- Mandatory fields are marked with colored background under their label.
- Changes may be abandoned or acknowledged with the OK, Cancel and Apply buttons.

Usage of record editors

At the top of the editor page, several tabs may be used to display a specific editor sheet which contains several data controls. These controls make it possible to display or edit the values of the data fields. A sample record editor page is shown for a specific Measurement entry. This property page helps to illustrate all important controls used on editor pages.

Several buttons are located at the bottom of the window. *OK* and the *Apply* button acknowledge changes, and store back the changed values to the database. The *OK* button also closes the window after a successful save. *Cancel* abandons the changes and closes the editor window.

The mandatory data fields are designated by different background colors under their labels. The roles of quick buttons beside the data fields are detailed below.

Quick buttons

On the right side of the edit boxes, various quick function buttons are placed.



The *record editor* buttons to edit the properties of the currently selected dependent item.

These are used extensively throughout the application, also on our Measurement record editor example. One such button is beside the field MEASURED BY. If you click this button, a new record editor form appears, containing details for the currently selected user: Database administrator.



The *new record creator* buttons are also used on most editor forms, and create a new dependent record. If you click this button beside the field MEASURED BY, a new record editor form appears, with a newly created Employee record.



The *reference remover* button removes a reference to a dependent item. It is displayed only for optional fields. For example, if you click on this button beside the field SOURCE, it clears the measurement's reference to any source, thus changing this field to empty value. The previously linked source record itself will not be modified.

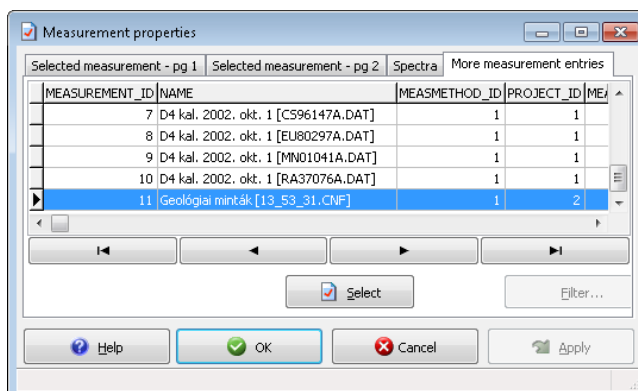


The *current date and time setter* button sets the value of the belonging date/time field to the current time.

Tab for additional records

The last tab of property editor pages lists additional records.

You can initiate the editing of any record, if you select it on the record list, and press the Select button.



2.3. Special property editors

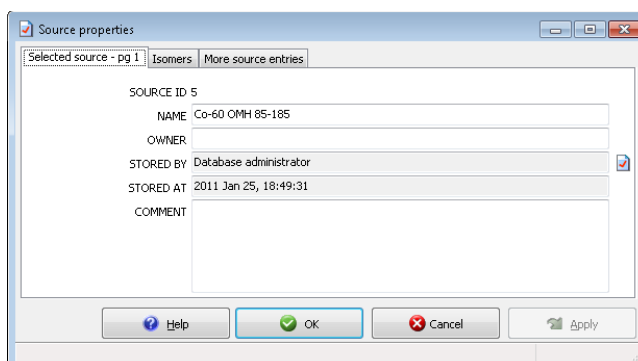
This section describes the property pages which may require some special usage instructions compared to the generic property pages.

2.3.1. Source properties editor window

The source properties editor page may be used to enter details for a newly created source record. Entries of radioactive sources keep together source and isotope information to use it effectively throughout HyperLab. Our example will discuss entering details for a new source entry, which belongs to a sample measurement, as detailed in section “Importing sample spectra”.

After you initiated the creation of a new source entry, the source editor window appears.

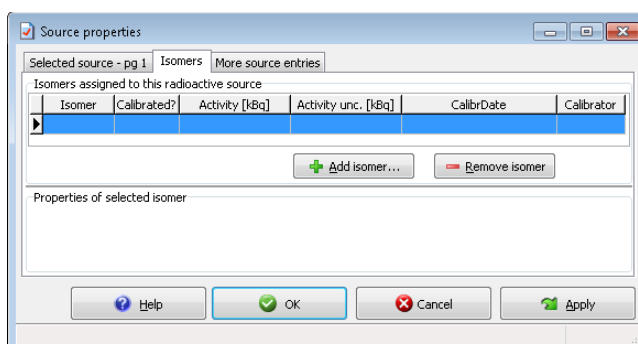
Specify a descriptive name for the source in the *Name* field, then click *Isomers* tab to define the contained isotopes.

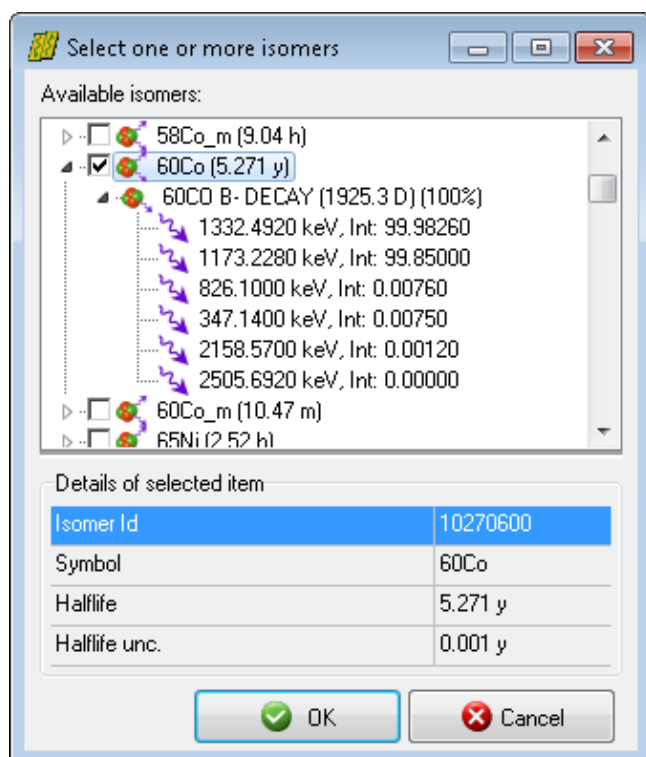


In HyperLab terminology, the source requires only the identification of isomers – and not the decays starting from that isomer level –, because it is always guaranteed that a source provides gamma radiations from all possible decays which are originated from an isomer state.

To add a new isomer entry to this source, click *Add isomer* button.

The isomer selector window appears now.

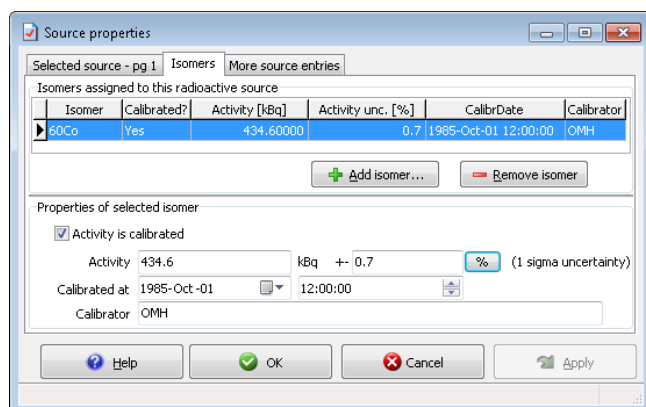




For our sample source, select ^{60}Co isomer with 5.27 year half-life. To speed up the selection process, quickly type in the first few letters of the isomer, and the list will scroll to the specified position.

You can also browse the decays and the associated gamma radiations for the isomers.

When you are ready, click OK.



The source editor's Isomer page appears again, and the list of assigned isomers contains the selected item. Now place a check "Activity is calibrated", and type in the certified calibration values.

For the "Co-60 OMH 85-185" source of the sample spectra set, specify 434.60 kBq activity and 0.7 % activity uncertainty, then 1 Oct 1985 12:00 as the calibration date.

Notes:

- Activity uncertainty has a unit changer button: this way you can specify it either in kBq (absolute uncertainty value), or in % (relative uncertainty value).
- Make sure that the entered uncertainty value corresponds to 1σ confidence limit, as the calibrator authority sometimes specifies it with 2σ . In this case you should enter half of the standard deviation value.

3. FWHM calibration

Before HyperLab performs peak evaluation of spectrum counts, at least a rough FWHM (Full Width at Half Maximum) calibration is necessary. Although HyperLab fits the width of peak, it requires a real estimation of the peak width, and it will allow to vary the fitted width from this initial value by a preset ratio.

FWHM calibration entries are created by the spectrum importer, when a proper calibration is loaded from the imported spectrum file. New calibration entries may be created by the user in the peak evaluator module.

3.1. FWHM calibration concept in HyperLab

In pre-2009 versions of HyperLab, the FWHM (Full Width at Half Maximum) was described with the following formula:

$$FWHM = \sqrt{A + B \cdot Ch}$$

and the resulting FWHM value was in channels. This expression depicts a linear dependence between the peaks' channel position (or energy) and their squared width.

This is proper for usual energy ranges (up to about 2MeV) and usual number of channels, but if you are utilizing broader energy ranges and/or many more channels, then significant differences start to emerge between the measured and predicted peak widths. Thus a more powerful FWHM function was introduced:

$$FWHM = \sqrt{\text{polynomial}(Ch)}$$

The meaning of this finer FWHM function remained the same: describes the FWHM in channels for any given channel value.

To create an FWHM calibration, users first specify several calibration points (channel values with belonging peak widths), and direct HyperLab to perform a least-squares fit to these data points, and determine the offset and slope parameters of the linear function, or the further polynomial parameters in case of the polynomial FWHM function. The linear function requires at least 2 calibration points, while the polynomial version requires $n+1$ points (n is the degree of the requested polynomial).

The FWHM calibration points as well as the fitted parameters are stored in HyperLab databases for each measurement entry. More than one FWHM calibrations may exist in the database for the same measurement, but only the last non-tentative one is treated as the current, valid FWHM calibration, and this will be automatically loaded by the peak evaluator.

The FWHM calibration editor is used to modify the values of the data points, to add or remove points, or to replace the current calibration with another from the database.

4. FWHM calibration editor

This window may be used to edit the calibration points of the FWHM calibration. For details about HyperLab's FWHM calibration concepts, see section “FWHM calibration”.

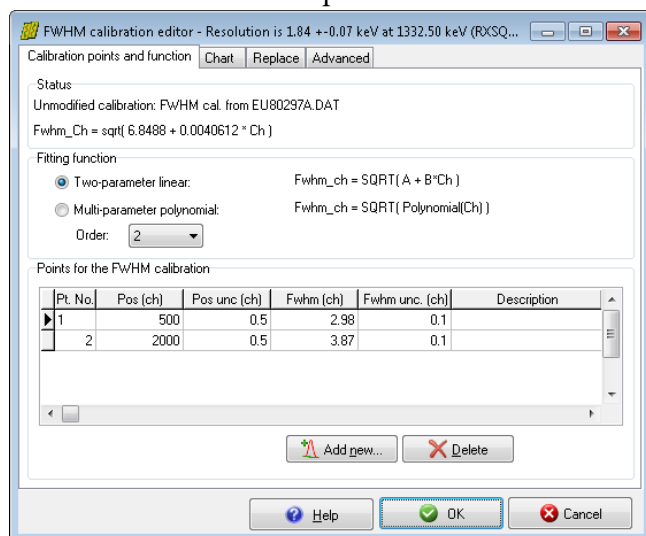
FWHM calibration window may initiated basically from two places:

- from the Spectrum peak evaluator. In this case, the primary purpose of the dialog is the editing of the calibration and especially adding new calibration points;
- from other places, e.g. from the spectrum importer, when the primary purpose of the window is to display a previous calibration in read-only mode.

This window contains multiple tabs with various data displaying or editing controls.

4.1. Basic FWHM editing operations

The first tab shows the input data for the calibration, as well as basic information about it.

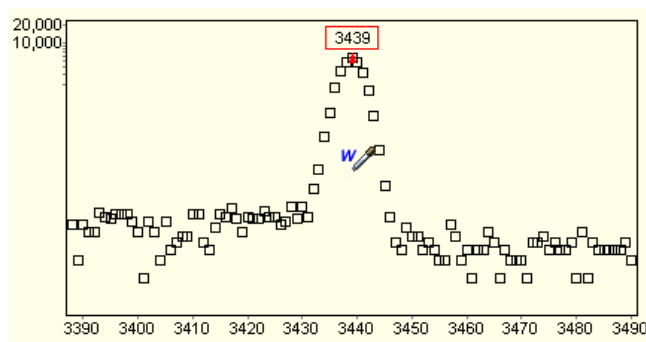


These comprise the current status (modified or unmodified), and the calibration point list as well. The point list contains two or more editable calibration points, to which a fit is performed, thus determining a FWHM calibration curve, which basically has a square-root shape, and serves FWHM in channel units.

If the fitting function is linear, then a *line* will be fit to square of the input FWHM values. If only two input points are used, the line must go through both points. If more than two input points are specified, a least-square fit is performed, in order to determine the optimum calibration line between scattering points.

If the fitting function is a polynomial, then a *polynomial curve* is fitted to the data points. This requires $n+1$ input data points, where n is the degree of the polynomial, and is advised only if you have experienced significant deviation from a simple square-root FWHM curve.

Adding new points by visual selection



HyperLab makes it possible to quickly add a new calibration point via a convenient method. If you click *Add new* button under the list of calibration points, HyperLab displays the spectrum evaluation window, where you can click above a spectrum peak to get its FWHM value.

You can use this feature both for unfitted counts (raw channel content, as seen on this figure) and above fitted peaks. After clicking, the position and width of the peak

will be used for a new FWHM calibration point. This way the addition of a new calibration point may be accomplished rather quickly.

Deleting points

To delete a specific FWHM calibration point, select it by clicking on it with the mouse, or make it active by pressing the up or down cursor arrow keys, and click *Delete* button.

FWHM chart for visual overview

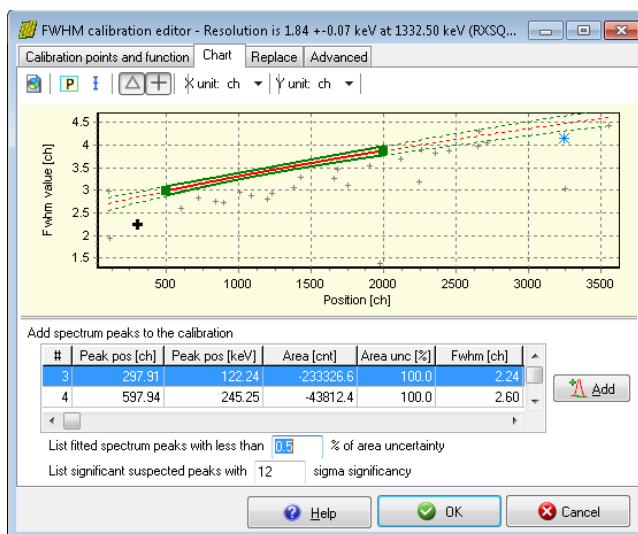
A very useful, quick, graphical overview of the current calibration may be found on the *Chart* tab.

The FWHM calibration curve is displayed as a red line. The solid red line shows the FWHM function between the first and last calibration points, while the dashed one shows extrapolated regions. The green lines above and below the red curve shows the $\pm 1\sigma$ uncertainties.

The calibration points which are actually used for the fitting of the FWHM curve are displayed as filled green squares.

The available peaks are displayed as gray cross (+), if not fitted yet in the spectrum, or with gray triangle (Δ), if the peak is already fitted.

The chart also shows a blue star symbol for orienting the user: this is theoretically the 'best' achievable resolution: 1.7 keV at 1332 keV energy. Peak labels are provided by the [P] button.



4.2. Example: correcting an improper FWHM calibration

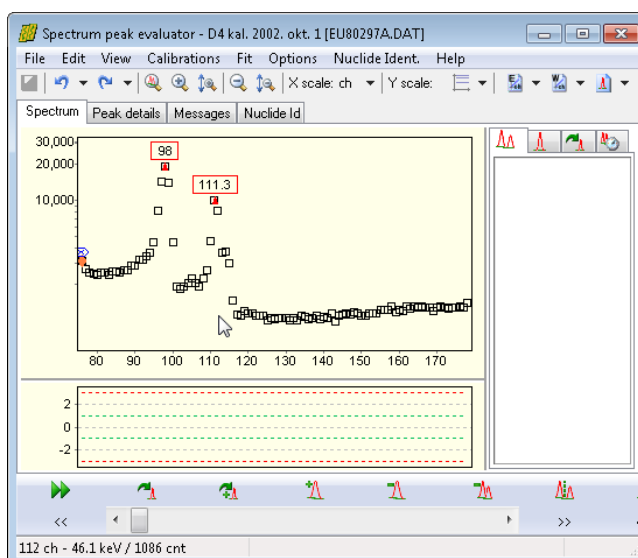
This section details the correction of a FWHM calibration, which was slightly off from the real value.

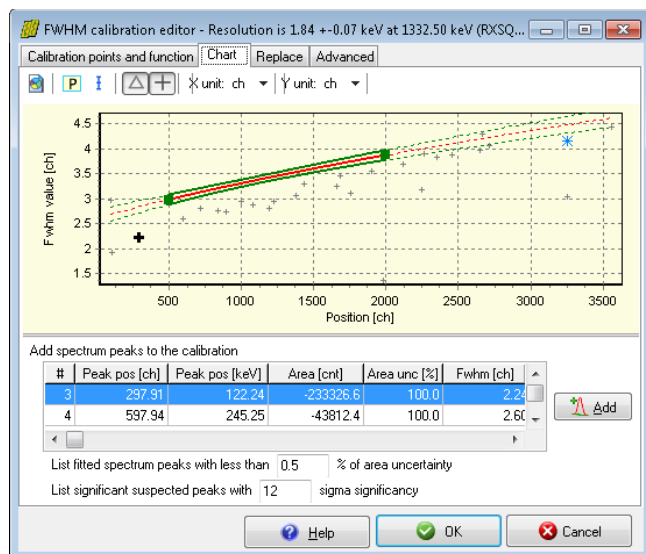
When a measurement is loaded into the peak evaluator, it is always advantageous to perform a quick check on the FWHM calibration before the spectrum deconvolution.

In order to get a visual overview of the current calibration, select *Calibrations / FWHM calibration* menu.

The FWHM Calibration Editor window appears now.

Click on the *Chart* tab.





By the help of the chart, one can immediately characterize the situation:

- numerous non-fitted (suspected) peak is available in the spectrum (gray + signs)
- the non-fitted peaks spreads nicely along a square-root-shaped curve, so the construction of the FWHM curve is expected to be an easy task
- no significant fitted peak is available at this moment (no gray Δ signs visible)
- the current calibration curve (continuous red line) is determined from two data points (green squares)

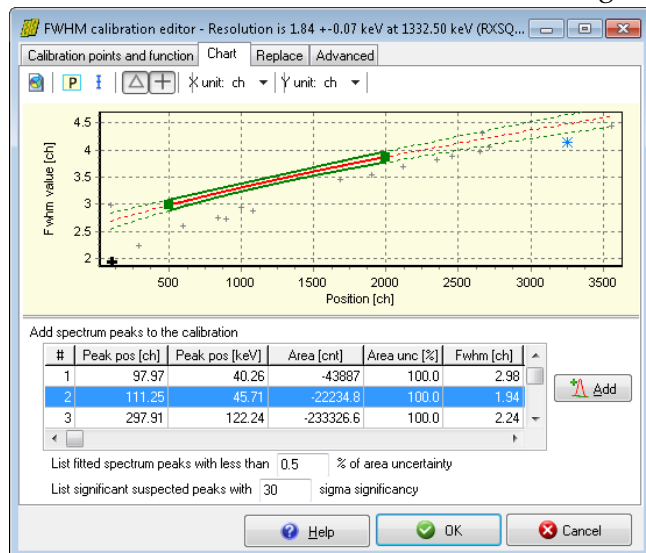
Also immediately can be seen that the current calibration curve is sub-optimal:

- the fitted FWHM curve differs significantly from the FWHM of the peaks (the red curve is above the gray crosses, especially in the low energy region): a slight mis-calibration is suspected,
- the energy range of all the peaks are not well covered by the FWHM curve; in other words, in wide regions only extrapolation is provided,
- only two calibration points have been utilized.

The solution for this problem should be the refinement of the current calibration points, and/or adding several ones in order to get a more relevant FWHM model.

Adding new points from list of available peaks

On the bottom of the Chart tab you can find the list of available peaks, which can be added to the FWHM calibration. This list contains the significant non-fitted and fitted peaks.



The list is filtered, so only the most relevant peaks (with the lowest area uncertainty) will be listed here. For non-fitted peaks the values will be estimated, and estimated peak areas displayed as negative values. First we increased the filter significance: entered 30 as sigma, in order to dismiss the uncertain, small peaks on the graph. Then we click over a proper candidate peak, and finally on the *Add* button. The selected peak will be added to the FWHM points, and the fit will be immediately performed.

After adding 4 FWHM points, the fitted curve does not really follow the new points, but keeps following the old ones.

In order to find out the reason for this, switch on the error bars by clicking on the error bar button at the top.

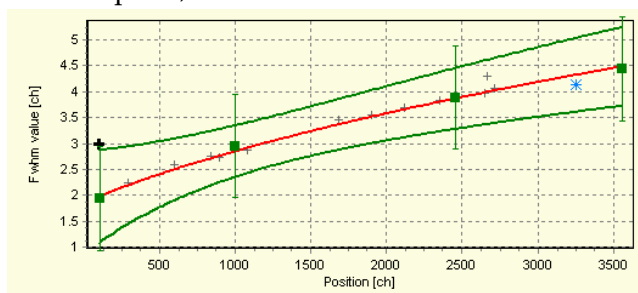
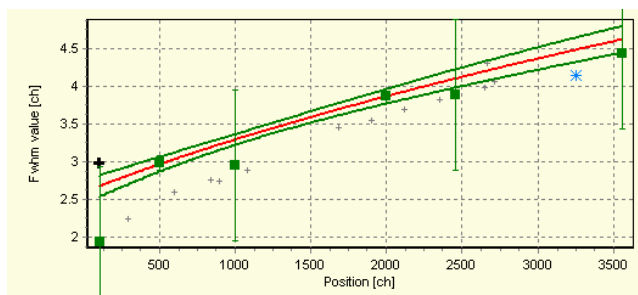
This immediately shows the root of the problem: the old calibration points – which are originating from the spectrum file – have too low FWHM uncertainties, thus their fitting weights are unreasonably high.

As those points seems to be rather inaccurate in all respects, we will delete them.

To delete a point from a chart, simply click on its green square. After the click, the first tab will be active, and the clicked point's corresponding row will be selected. Now click the *Delete* button, thus remove the point from the fit.

After deleting the two original calibration points, the fitted FWHM curve reasonably well describes the measured points, so you can acknowledge it by clicking on the *OK* button, and perform the whole-spectrum deconvolution.

Please note that HyperLab's spectrum fitter requires only a *rough, approximate* FWHM calibration, as it allows the peak width to vary by 30% from the FWHM calibration during the nonlinear fit. Nevertheless, a quick overview of the FWHM calibration is always advisable before fitting.



4.3. Advanced FWHM editing

Entering new points manually

If you do not want to use HyperLab's visual calibration point adding facility, just want to enter predefined calibration points, press the ↓ (cursor down) key repeatedly, while you leave the last point's row, and a new, empty row automatically created. Type in the proper values, then press ↑ (cursor up) key to leave the edited calibration point row. If you want to enter a completely new calibration, first remove all calibration points, then the add them one by one.

Modifying channel positions

To modify the channel position of a specific calibration point, you have two options: manual editing or borrowing.

To edit the value by hand, just click on the channel number value, and type the new number. To borrow, you should use the borrow button of the FWHM field.

Points for the FWHM calibration				
Pt. No.	Pos (ch)	Pos unc (ch)	Fwhm (ch)	F
1	111.25	0.5	1.94	
2	3560.76	0.5	4.44	

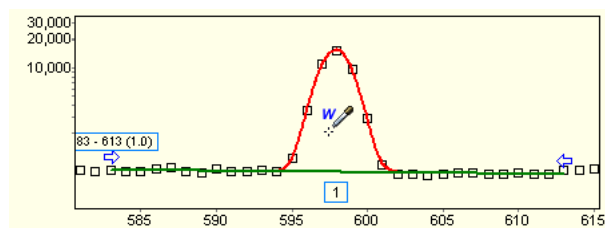
Modifying FWHM value of an existing calibration point

FWHM values may also be modified by either manual editing, or by getting the exact fitted FWHM values from the active HyperLab spectrum. This may be required if you modified the fit of a peak, which is used for FWHM calibration. Manual editing may be initiated by simply clicking on an FWHM value and typing its new value in channels.

Points for the FWHM calibration

Pt. No.	Pos (ch)	Pos unc (ch)	Fwhm (ch)	F
1	111.25	0.5	1.94	...
2	3560.76	0.5	4.44	
3	2454.41	0.5	3.88	

If you want to borrow a fitted peak width value from the current spectrum, click on the FWHM value, then on the ellipsis [...] button appearing beside the number.



The spectrum fitting window appears now. Click with the position getting tool on a peak. The FWHM calibration editor will appear again, and the clicked peak's exact fitted peak width will be used as the FWHM value of the calibration point.

Should you want to cancel the borrowing process, press *Esc* key.

Please note that, after borrowing, the channel position of the FWHM point is also updated to the position of the fitted peak. This behavior is intentionally different from what you experience in the case of the energy calibration editor.

5. Energy calibration

After HyperLab's spectrum peak evaluator determined the position and the area of the peaks, it creates a peak list, where the peak centroids are shown both in channel and in energy (keV) unit. The energy values are calculated from the fitted channel values by utilizing the energy calibration function, which performs this transformation.

HyperLab's energy calibration function is different from most competitors' solution: it uses a simple linear channel – energy function with an optional additive nonlinearity function.

When nonlinearity is not used, energy values in keV are computed from the channel values with the following formula:

$$E = A + B \cdot Ch$$

When nonlinearity correction is in effect, that function will always provide the higher order terms for the channel vs. energy function:

$$E = A + B \cdot (Ch + NonlinShift)$$

This second formula contains the *NonlinShift* parameter, which is computed from the system's nonlinearity curve, and is a polynomial of the channel value.

5.1. Linear and nonlinear calibration

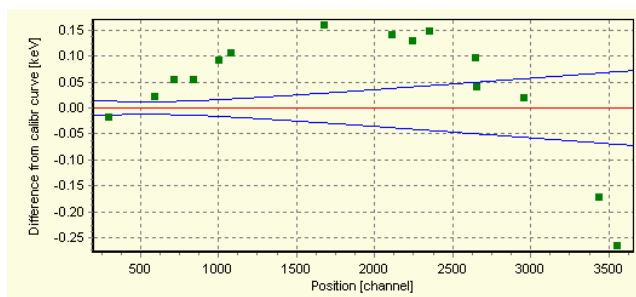
In most cases, a simple linear channel – energy function is not acceptable for post-processing, as this would lead to two adverse effects:

- **Inexact energy positions.** This is due the inherent nonlinearity of the measurement systems, and finally would cause improper nuclide identification in post-processing of the peak lists. If nonlinearity correction is not applied – that is, solely the linear calibration function is used – peak positions of the fitted peak positions may differ as much as 1-3 channels from their expected value.
- **Improper uncertainties.** If only the linear calibration function is used, the reported uncertainties on peak positions are smaller than the real values, thus would make the isotope identification unreliable for activity calculation and calibration purposes.

This picture shows the case when only a linear energy calibration is used for a typical measurement system. This is a measurement of a ^{152}Eu source, in the 121 keV – 1408 keV range.

The green squares depict the difference (the residual) of the calibration points' position from the linear calibration (red line).

Despite multiple calibration points, a clear tendency shows that the system has a significant nonlinear response, which reaches several tenths keV at in the vicinity of 1408 keV.



If these discrepancies are not acceptable, the purely linear energy calibration is not enough: a correction is needed to eliminate the nonlinearity of the measurement system.

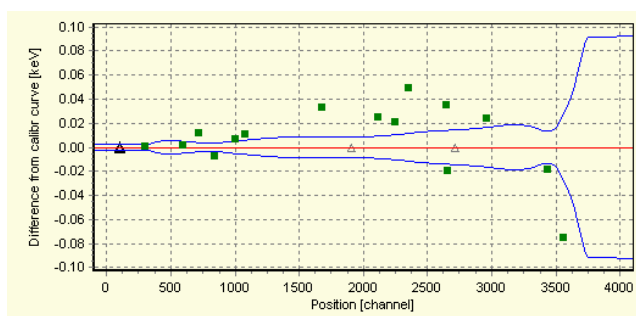
5.2. The energy calibration concept in HyperLab

A basic assumption of HyperLab is that every measurement system has an inherent and characteristic nonlinearity, which is rarely and slowly varying in time. We also assume that this is very different from the daily shift of the linear calibration values, and may be separated from it. Thus the nonlinearity function should only be determined occasionally, e.g. with a multi-isotope, multi-measurement calibration set, providing a high precision nonlinearity curve. This nonlinearity curve can be used in the daily work for a longer period – e.g. for a half year or a whole year –, and only the linear part of the calibration should be adjusted daily.

This way a convenient and high-precision energy calibration is achieved by minimum amount of work.

This figure shows the effect of applying a real nonlinearity curve in addition to the same linear calibration as seen on the figure in section “Linear and nonlinear calibration”.

Please note that the nonlinearity virtually disappeared throughout the whole energy range, and one magnitude smaller unwanted shifts may be observed in peak positions (hundredths of keV).



As you can see the abrupt change of the blue $\pm 1\sigma$ error curve after the last calibration point, HyperLab does not allow nonlinearity curves to be used for extrapolation. When a nonlinearity value is requested for an energy, which is outside the energy range of the nonlinearity calibration, the nonlinearity value of the first or last point will be used instead.

Further benefits

By utilizing a separated nonlinearity curve for the system, it also provides further benefits:

- the uncertainty calculation contains the incremental effect of the system nonlinearity, and
- it is possible to apply the precise nonlinearity even when the spectrum has a small number of calibration peaks.

As the nonlinearity calibration takes only a few minutes to create, and provides peak positions with much higher precision, our advice is to *always* use the nonlinearity part of energy calibration.

In fact, this process is almost fully automatic: during loading a spectrum file, HyperLab is able to assign the actual nonlinearity curve to the measurement's energy calibration. After this step, all computations involving this energy calibration will automatically utilize the compensation.

5.3. Energy calibration editor

This window may be used to edit the calibration points of the linear energy calibration part, and also to select an additive nonlinear energy calibration curve to the calibration. For details about HyperLab's energy calibration concepts, see section "Energy calibration".

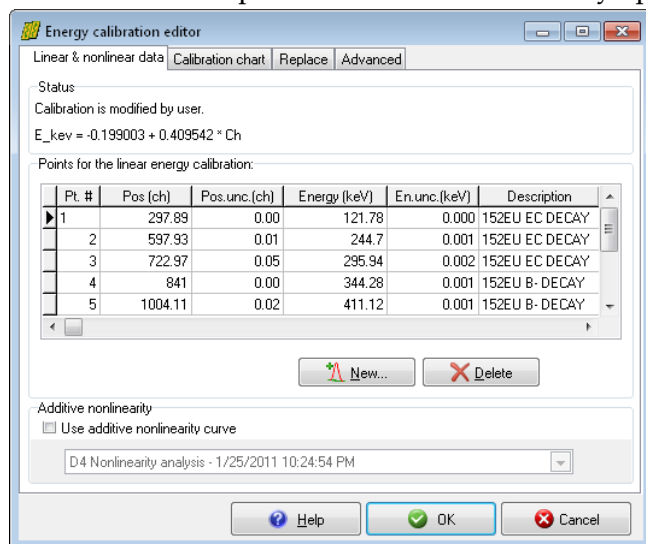
The energy calibration window may be initiated basically from two places:

- from the Spectrum peak evaluator. In this case, the primary purpose of the dialog is the editing of the calibration and especially adding new calibration points;
- from other places, e.g. from the spectrum importer, when the primary purpose of the window is to display a previous calibration in read-only mode.

This window contains multiple tabs with various data displaying or editing controls.

5.3.1. Linear and nonlinear data tab

This tab contains all the data necessary for quick overview of the calibration's most important numeric data. These comprise the current status (modified or unmodified), the calibration point list as well as the optional additive nonlinearity applied.



The point list contains two or more editable calibration points, to which a linear fit is performed, thus determining a channel – keV calibration line. If only two points are used, the line will necessarily go through the points. If more than two points are specified, a least-square fit is performed, in order to determine the optimum calibration line between scattering points.

The nonlinearity curve provides a fine tuning, to compensate system nonlinearity. See further details in section "System nonlinearity analysis".

Deleting points

To delete a specific calibration point, select it by clicking on it with the mouse, or make it active by pressing the up or down cursor arrow keys, and click *Delete* button.

Entering new points manually

If you do not want to use HyperLab's visual calibration point adding facility, just want to enter predefined calibration points, press the ↓ (cursor down) key repeatedly, while you leave the last point's row, and a new, empty row automatically created. Type in the proper values, then press ↑ (cursor up) key to leave the edited calibration point row. If you want to enter a completely new calibration, first remove all calibration points, and add them one by one.

Modifying channel positions

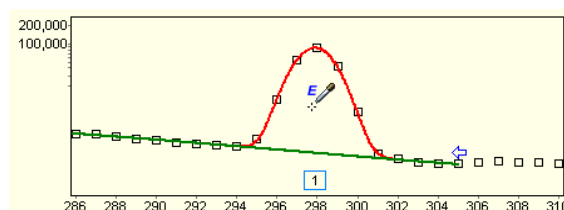
To modify the channel position of a specific point, manual editing or borrowing may be used.

To edit the value by hand, just click on the channel number value, and type the new number. To borrow the exact peak position value from a fitted spectrum peak, click the ellipsis [...] button beside the channel value.

Points for the linear energy calibration:

Pt. #	Pos (ch)	Pos.unc.(ch)	Energy (keV)
1	297.89	0.00	121.78
2	597.93	0.01	244.7

The spectrum fitting window appears now. Click with the position retrieval tool on a peak. The energy calibration editor appears again, and the clicked peak's fitted position will be used as the channel value of the calibration point. To cancel the borrowing process, press Esc.



Modifying energy values

Similarly to channels, energy values may also be modified by either manual editing, or by getting the exact values from HyperLab's nuclear data database. Manual editing may be initiated by simply clicking on an energy value and typing its new energy position in keV.

If you want to use a value from the nuclear database, click on the energy value, then on the ellipsis [...] button beside the energy value.

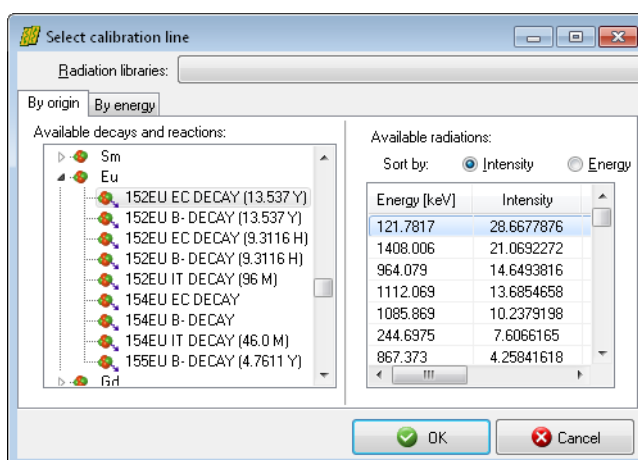
Points for the linear energy calibration:

Pt. #	Pos (ch)	Pos.unc.(ch)	Energy (keV)
1	297.89	0.00	121.7817
2	597.93	0.01	244.7

The *calibration line selector window* appears now. It contains decays and radiations from the database.

When this window first appears, you can type in the first letters of the element, when the decay lister will select the appropriate element. After the element is selected, open it by clicking on the [+] at the left to show up its decays. Now click on one decay and its radiations will be listed on the right.

To select a radiation, click its line in the *Available radiations* table, then click OK. Alternatively, you can simply double-click on the radiation's data row.



The radiation list can be sorted by the *Intensity* and the *Energy* radio buttons at the top of the list as required. When you selected an energy row, the energy calibration editor window appears again, displaying the modified energy value.

Adding new points by visual selection

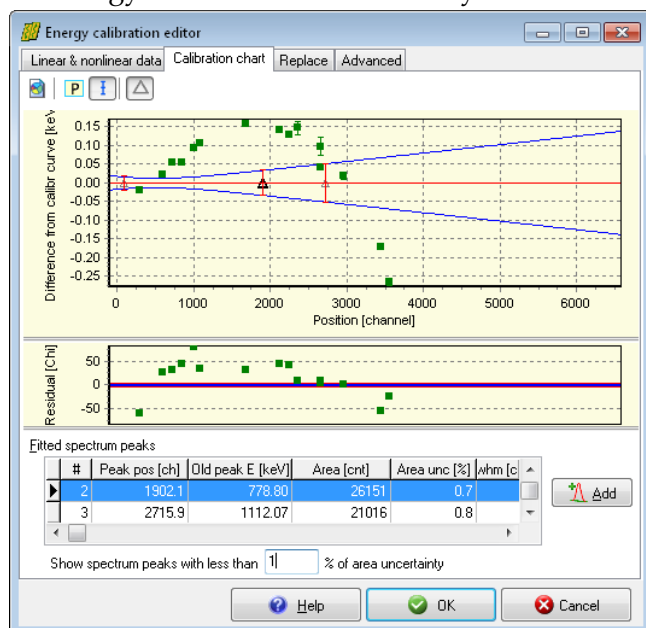
HyperLab also makes it possible to add a new calibration point via a more convenient method. If you click *New* button under the table of calibration points, HyperLab first displays the spectrum evaluation window, where you can select a fitted peak for position, then instantly shows the *calibration line selector window*, in order to select a calibration line from the nuclear database. This way addition of a new calibration point may be accomplished rather quickly.

The problem of missing gamma lines

It may be disturbing that some of your well-known calibration peaks are not provided in the calibration line selector window. This may be due to its missing *radiation usage flag*. HyperLab uses a gamma line for energy calibration purposes only if that radiation is equipped with “Use for energy calibration” flag. See further details in section Nuclear data library management.

5.3.2. Calibration chart tab

The energy calibration chart allows you to overview the quality of the calibration.



This sheet contains the chart itself at the top, a residual at middle, and a list of candidate fitted peaks at the bottom. The chart shows the *calibration line* with red, the *standard uncertainty* of the calculated energy values in blue; the calibration points' *difference* from the energy calibration line as filled green rectangles.

The peak list may be used to add new points quickly to the calibration. The peak list is filtered to display the significant peaks only: only the peaks with less than 1% peak area uncertainty will be displayed – however, this value can be edited under the list. If you find too few peaks in the list, change this value to, say, 5%, and all the peaks below this limit will be listed immediately. To quickly *add a peak* to the

calibration as a new point, click on its row, and click the *Add* button beside the list.

On the chart, gray triangles depict the positions of the fitted candidate peaks, which are listed in the peak list table. When you click on a gray triangle, its point will be shown with bolder line, and the corresponding data row will be selected. The fitted peaks are always displayed with zero difference from the calibration curve, as their library energy is not yet known. When Add button clicked, user should select a library peak, then a real difference may be computed.

Notes:

- The gray triangles may help you to notify if you are using dangerous extrapolation: if the last fitted peak – that is, the last gray triangle – is too far from the last green calibration point, its computed energy value may be rather uncertain. In this case, it is advisable to add also another, closer peak as an additional calibration point.
- If you see a strong non-random tendency among the linear calibration points, and the difference exceeds, say, 0.1keV, this may indicate significant nonlinearity of your measurement system. In this case, it is advisable to create a nonlinearity calibration, and use it together with the two-point linear energy calibration as a nonlinearity compensation. See details in section “System nonlinearity analysis”.

5.3.3. Advanced tab of energy calibration window

On the advanced tab, you can revise the equations of the current energy calibration. If the additive nonlinearity correction is not used for a given calibration, then a simple

$$E = A + B \cdot Ch$$

formula is used. In case of nonlinearity correction, the

$$E = A + B \cdot (Ch + NonlinShift)$$

formula will be applied, where *NonlinShift* is computed from the polynomial of nonlinearity curve for a given channel value.

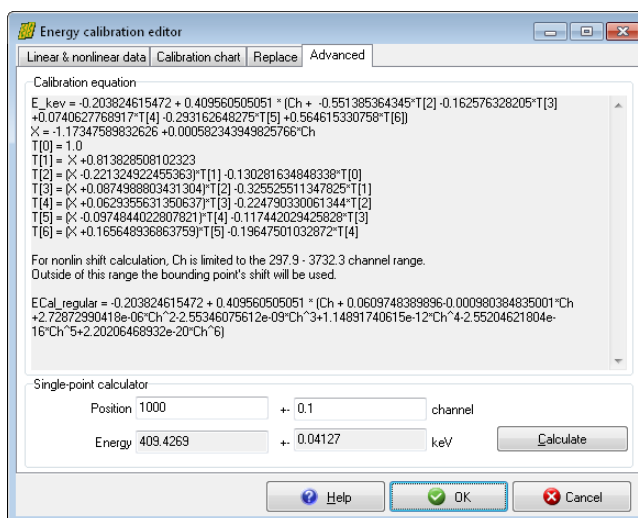
This should result in much better agreement of the measured peak positions throughout the whole measurement range. The calibration chart will also significantly change: calibration points will scatter randomly around the calibration line, and the differences between the points and the line become much smaller, thus resulting in much more precise peak position determination.

This tab displays the energy calibration function in two forms.

The upper part contains the exact and numerically stable representation, which utilizes orthogonal polynomials. This solution, however, may seem uncommon.

The lower part displays the very same function as a regular polynomial, whose computation is more straightforward. It may be used in external applications, where the simplicity has higher priority than numerical stability.

This page also makes it possible the computation of any energy value and its uncertainty from arbitrary channel values: just enter the position in channels into *Position* edit box, and possibly its absolute 1σ uncertainty. Upon clicking Calculate button, the corresponding energy value will be displayed, together with its absolute uncertainty value.

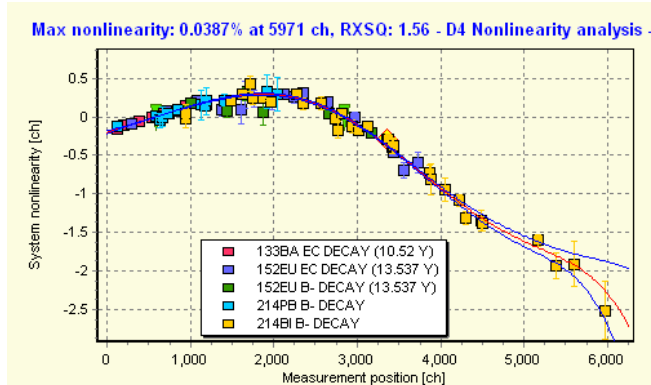


6. System nonlinearity analysis

As described in section “Energy calibration”, HyperLab proposes an energy calibration model, where the slowly varying nonlinear and frequently changing linear parts are separated.

Nonlinearity curve

The nonlinearity of a measurement system at a specific point of time is characterized by a so called *nonlinearity curve*. This describes the system's *deviation* from the linear calibration line, as shown in the picture below.



The figure shows the nonlinearity curve of HyperLab's Nonlinearity module for several calibration measurements.

The curve itself is depicted by a red line, its $\pm 1\sigma$ limit with blue lines, while the data points are from the centroid shift of the fitted peaks.

The green triangles (at 600ch and 2800ch) show the points where the curve crosses the zero nonlinearity value.

In HyperLab, the system nonlinearity curve always uses the channel-channel scale, as

with these units the nonlinearity characteristics are supposed to be slowly varying with the time.

The calculated nonlinearity may be used for several purposes:

- The curve provides the “fine tuning” part of the energy calibration, because it transforms the system's response to nearly linear. Thus, when applied together with a linear channel-position calibration line, it serves more exact energy values. See section “Energy calibration editor” for more details about applying a previously created nonlinearity calibration to an existing linear energy calibration.
- Helps to compare the absolute nonlinearity of different measurement systems. As HyperLab also calculates an absolute percentage nonlinearity value, a simple comparison of two numbers may reveal the differences between them.
- Helps to characterize the aging or other changes in a specific measurement system for quality assurance purposes. With consecutive nonlinearity evaluations, the percentage nonlinearity values may be used to monitor the changes in characteristics of the measurement system.

6.1. Algorithm of nonlinearity determination

Nonlinearity determination is easy with HyperLab's Nonlinearity module. Only a few measurements are required, and a calibration curve may be constructed within a few minutes.

The algorithm of the nonlinearity determination is the following:

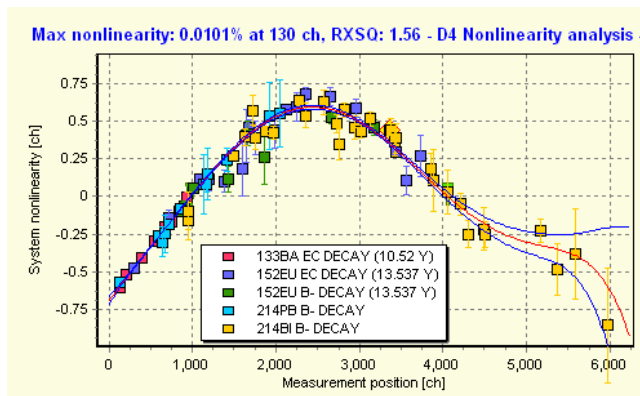
1. Determination of the matching gamma lines in the measurements. Because 2 parameters will be determined during a least-squares fit for each measurement, this step drops measurements with less than 3 matching data points.
2. One-step fit performed on all points of all measurements with one common orthogonalized polynomial, and with more adjusting lines, one for each measurement. The shape of the polynomial describes the common nonlinearity in the system, while the lines normalize together the individual measurements so that the common chi-squared is at the minimum.
3. As the nonlinearity of the system is described practically only by the curvature, a final common shifting line is added, which may be arbitrarily chosen by the user.

6.1.1. Nonlinearity intersection points

The additive line – the zeroth and first order member of the nonlinearity – is to shift or “shear” the curve such that it intersects the X axis at two specific points (where zero nonlinearity is reached, as shown by the green triangles).

The user can select from *Optimum*, *Linear fit* or *User defined* intersection (or *baseline*) determination modes. The figure shows the same nonlinearity analysis as in section “Nonlinearity curve”, but with *Optimum* baseline instead of *Linear fit*.

HyperLab uses the *Optimum* mode by default, because in this case the maximum absolute deviance from zero nonlinearity is minimized in the whole energy range.



The *Linear fit* option will use no additive line (or, equivalently it uses the first measurements' line – as it is selected as zero slope and offset).

In *User defined* mode the user is able to set her own intersection points (thus defining the additional line).

Notes:

- If you want to compare percentage nonlinearity values of different measurement systems, or the overall goodness of the same system at two different times, use *Optimum* method, because this provides the smallest possible percentage value.
- If you want to compare the shape of nonlinearity of two systems, apply *User defined* mode, and set intersection to the same values. This way the same shifting is applied to the curves, and their differences in shape will be immediately visible.
- If you want to check whether a linear energy calibration gives the same deviations from the calibration curve as the points on the nonlinearity curve, use *Linear fit* method with one single measurement.
- For energy calibration purposes, in essence there is no big difference between the methods, as the line of the linear energy calibration is able to compensate any setting of baseline. We suggest using the *Optimum* or *Linear fit* method in this case.

Bug note: a rarely occurring bug exists in HyperLab's minimax intersection determination algorithm. If you have a measurement system which has a nearly linear response almost in the whole range, the minimax fit sometimes results in the same intersection values for both intersection points. This is indicated by the nonlinearity display: only one green intersection triangle is visible instead of two, because they are at the same position. In this rare case please use the *Linear fit* or the *User defined* method.

6.2. Measurements required for nonlinearity determination

For nonlinearity determination, you need one or more multi-line measurements. The measurements should have the following properties:

- taken with the same measurement setup (same detector, ADC, energy range),
- taken roughly in the same time period (preferably within the same day, or within 1 week),
- their gamma lines of isotopes have exact energy values in HyperLab's database,
- the lines of the isotopes spread across your entire, regularly used energy range,
- every measurement has at least 3 proper gamma lines,

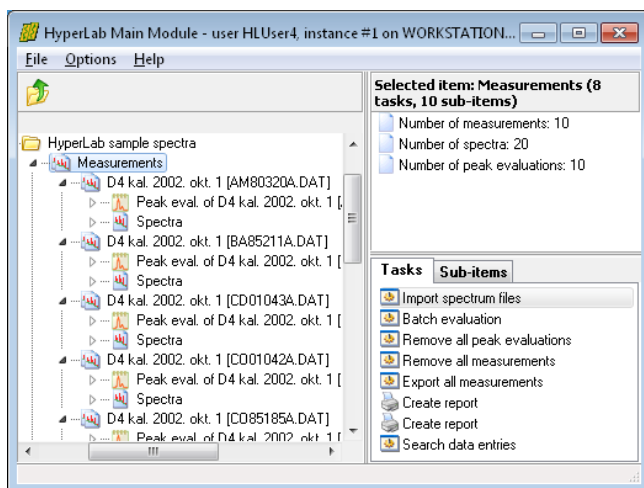
- every measurement has at least 2-3 identified peaks which *overlaps* with another measurements' identified peaks. Please be aware that if no overlapping is between the measurements, no proper nonlinearity curve may be constructed.

These are not stringent requirements, so the majority of usual calibration measurements – or even measurements acquired for material analysis – will be usable also for nonlinearity determination. You can also use isotopes with a few problematic lines, as you will be able to individually remove the disturbing or overlapping lines from the nonlinearity curve.

6.3. Steps of nonlinearity determination

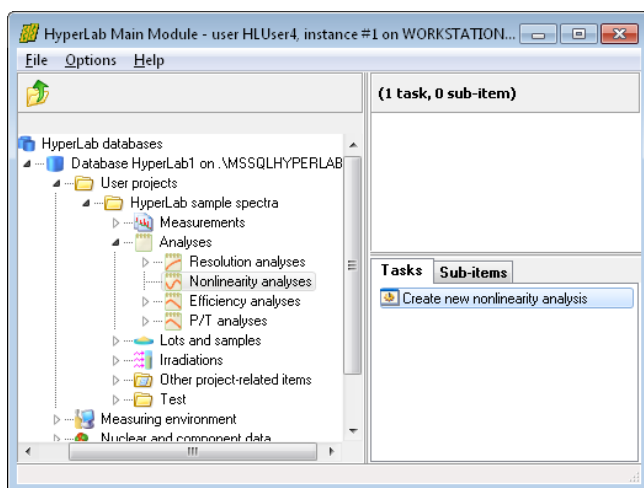
In order to determine the nonlinearity curve of a measurement system, first take some measurements with calibration sources, and import them into your HyperLab database. Our example will work with HyperLab's sample spectra belonging a measurement setup with 70 keV - 3300 keV range.

Please load the spectrum files into the database and also set their corresponding source values, as specified in section “Importing sample spectra”.



Perform a batch or individual evaluation on all measurements, and open a multi-line spectrum with the Peak evaluator. Check the FWHM calibration, and adjust the region fits, if necessary. Finally save the peak list, which will be input for the nonlinearity evaluation.

When all measurement are properly fitted, similar statistics will be displayed about them at the right side of the Main Module window as you can see in this picture.



Open *Analyses* node under your project, then click on *Nonlinearity analyses* and select Create a new nonlinearity analysis task.

A new window appears now, where basic parameters of nonlinearity fit algorithm may be specified.

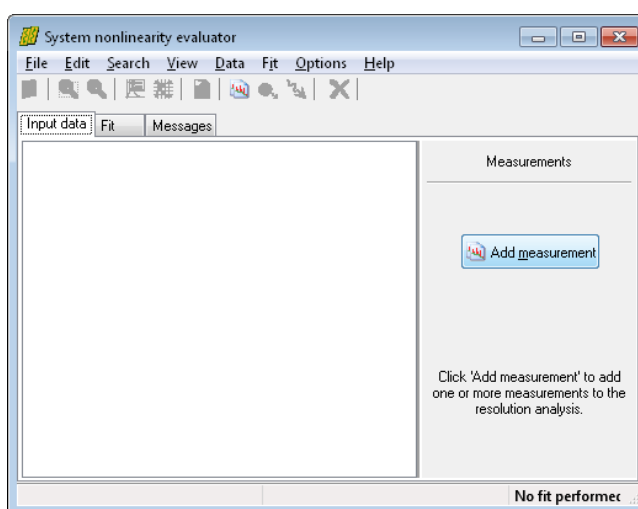
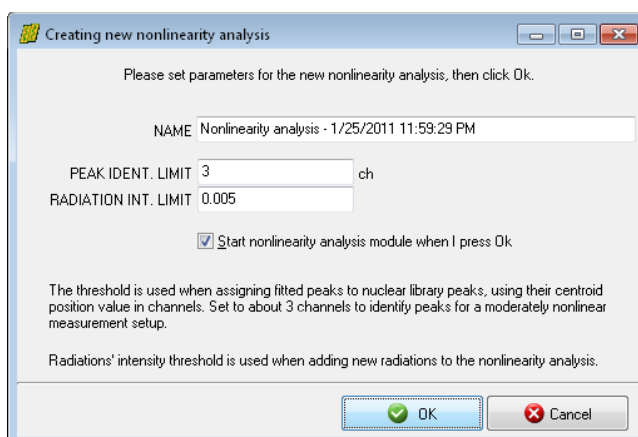
You can specify a descriptive name of the new nonlinearity analysis, and thresholds for the identification of peaks.

The *Peak identification limit* is used when peaklist peaks and nuclear library peaks are matched. If the difference between peak centroids is below this value, the peaks will be considered as matching. Its usual value is 3 channels, which is appropriate for measurement setups with moderate nonlinearity.

The *Radiation intensity limit* is used when radiations are loaded for a selected decay from the database. The 0.005 default value load the radiations where the intensity is greater than 0.5% of the decay's strongest line. When you are ready, press OK.

The *Nonlinearity evaluator* appears now with the empty *Input data* sheet.

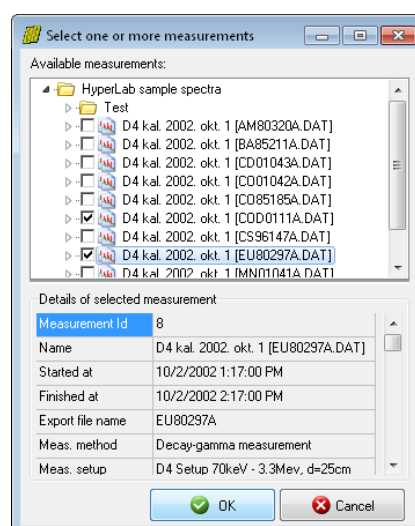
Click *Add measurement* button at the right. The *Measurement selector* window appears now.

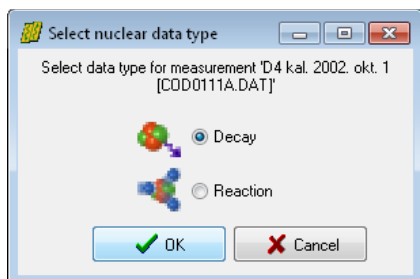


Select the ⁵⁶Co sample measurement from the project, named *COD0111A.DAT*, and ¹⁵²Eu measurement called *EU80297A.DAT*.

When you click OK in the measurement selector window, HyperLab performs the steps as follows.

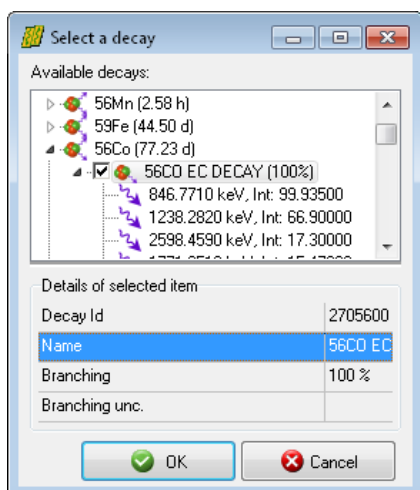
- Loads the peaks from the most recent peak evaluation of the measurement.
- Checks if a source is specified for the measurement. If found, loads the source isomers, their decays and radiations. Otherwise prompt the user for the isotopes.
- Limits the radiations to those whose intensity is above the preset intensity limit and which have a radiation usage flag stating that the radiation is usable for nonlinearity evaluations.
- Matches the loaded radiations and peaks, by applying the preset matching limit.
- If at least 3 matching peak-radiation pairs are found within a peak list, the measurement will be used for nonlinearity evaluation, otherwise skipped.
- Checks if enough input data points exist for a polynomial fit. The number of all data points must exceed the number of fitted parameters, which added from the degree of fitting polynomial and the two linear shifting parameters for each measurement.





If you did not specify the radioactive source for the ^{56}Co measurement, a selector windows will pop up now.

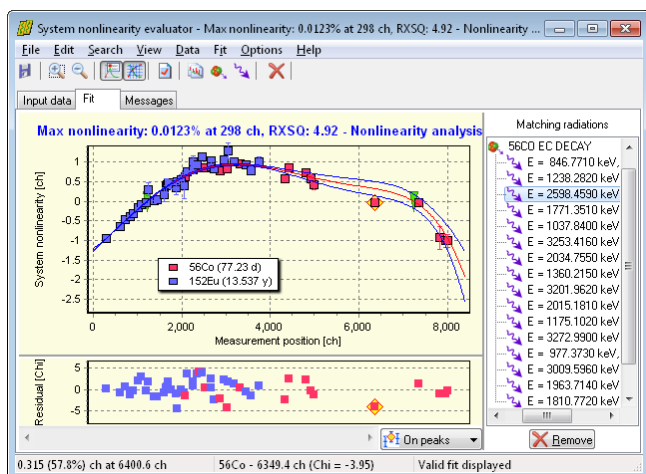
Select *Decay* option and click OK, as you are specifying a decay gamma source.



Next window let you select one or more decays for the given measurement. The gamma lines belonging to the decay is also listed, in order to help the selection.

Select *56Co EC Decay* entry, and lick OK.

If you did not specify the radioactive source for the ^{152}Eu measurement, repeat the process accordingly, and select both the EC and the β^- decays of ^{152}Eu .



If enough data points are supplied, the fit is performed and the tab Fit becomes active, displaying the fitted nonlinearity curve. Now you can add your other measurements to the fit one-by-one, or remove one, drop outlier gamma lines and so on.

Eventually, a multi-isotope nonlinearity curve may be constructed with almost no manual interaction.

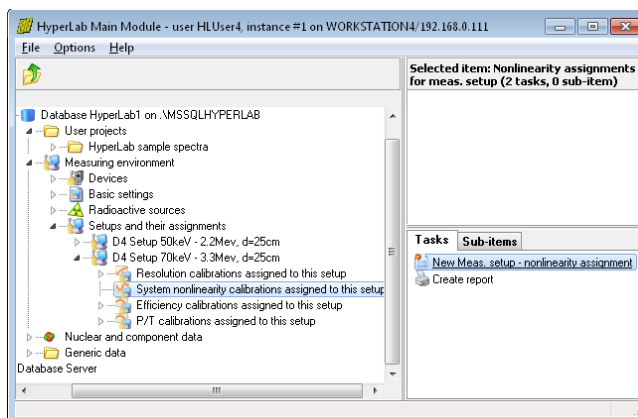
Note: after you are using a specific peak evaluation for nonlinearity analysis, you had better *not modify* the peak evaluation afterwards – e.g. by adding or removing peaks from it. When you open such a peak evaluation with the spectrum evaluator module, it will warn you about this, suggesting opening the evaluation only in read-only mode.

If you want to use a measurement for multiple purposes, e.g. for nonlinearity as well as efficiency analysis or quantitative evaluation, it is advisable to create a separate peak evaluation for each purpose, e.g. by cloning the original peak evaluation.

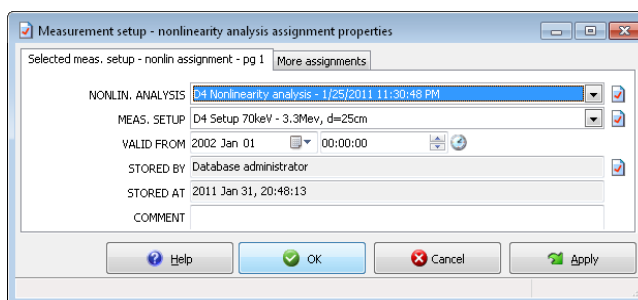
6.4. Designating a proper nonlinearity curve as a default

After a successfully construction of a nonlinearity curve, you should take one last administrative step: HyperLab should know that this curve is to be used as a default one. This can be done by assigning the nonlinearity analysis to the measurement setup where it belongs. After this step, the spectrum files, which loaded next time, may get this nonlinearity correction automatically, so your energy calibrations will be more precise right after the importing.

Open *Measuring environment* node in your database browser tree, then *Setups and their assignments*, finally the measurement setup where your nonlinearity curve is created. In our example, the measurement setup 'D4 Setup 70keV - 3.3Mev, d=25cm' was opened. After that entry, click *System nonlinearity calibrations assigned to this setup*, and then select the task at the right named 'New Meas. Setup – nonlinearity assignment'. A data entry window appears now.



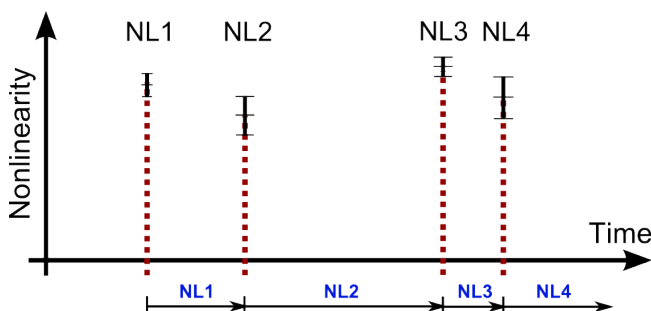
Now you should select the nonlinearity analysis you have created. Another important field is the *Valid from* entry, where you can define the starting date when your nonlinearity analysis should be used as a default. Set it to the **date of the measurements** which have been used for the analysis.



In our example, we set this date to January 1st, 2002, to make sure that it will be automatically used for all measurements taken from the very first day of that year.

You should always register a successfully created analysis as default. This way a chain of nonlinearity analyzes will be created, each representing a time range of your measurement system, when that calibration was valid.

On this picture we depict a situation, when 4 nonlinearity analysis, NL1, ... NL4 is determined for a measurement setup. After the first assignment (NL1), there is always a valid nonlinearity in the system. For example, if a spectrum file is imported, where the acquisition time is between the 2nd and the 3rd nonlinearity analysis, then the NL2 nonlinearity will be assigned to the energy calibration of that measurement during the importing.



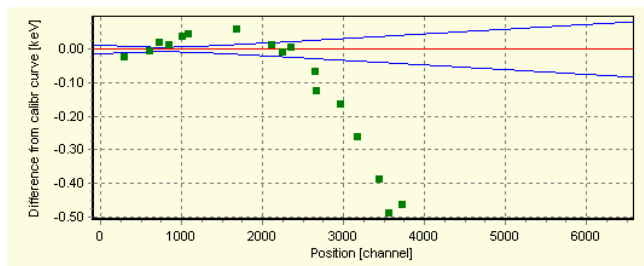
6.5. Common problems during nonlinearity determination

Although nonlinearity determination is almost a trivial task with HyperLab, there may be common problems for the users.

Problem No.1: improper linear energy calibration of measurements

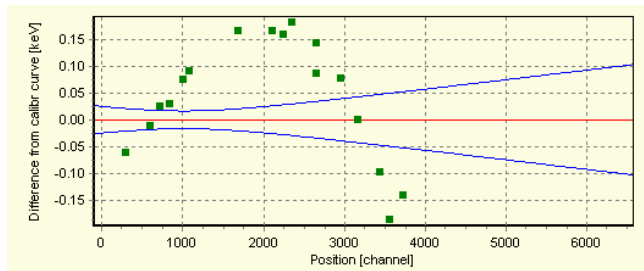
Perhaps the most important thing is to create a proper linear energy calibration for the measurements which will be used as input for the nonlinearity analysis.

The difference between the reported peak positions and the position of the library peaks at the end must not be larger than 3 channels (the actual nonlinearity peak search limit), otherwise nonlinearity module will not be able to find them.



In case of an improper linear energy calibration, as it is shown in this picture, the user forgot to use the high-energy lines of ^{152}Eu for the linear calibration.

These lines possibly will not be found by the nonlinearity analyzer, thus 'drawing off' the nonlinearity curve.



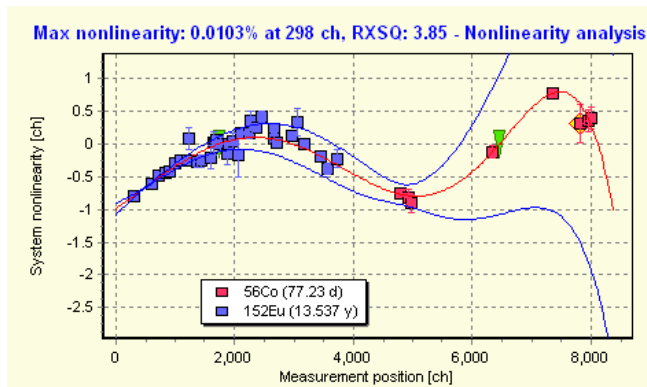
This figure shows a much better linear energy calibration for the same situation. You can see that the calibration line placed such way that no any library lines is located too far away from the actual peaks.

This way the nonlinearity analyzer will probably be able to find those peaks and incorporate them onto the nonlinearity

curve.

Problem No.2: non-overlapping regions covered by measurements

For nonlinearity fitting, the input measurements should contain as much well-defined singlet peaks as possible, as this makes it possible to describe well the shape of the nonlinearity curve. Please keep in mind that another important constraint for the analysis is that the final curve must be constructed from measurements where the peaks are overlapping each other.



This is because the fitting algorithm has the freedom to rotate the curve part freely, in order to get a joint with minimum overall nonlinearity.

Please take a look at this faulty multi-isotope nonlinearity curve constructed from the two overlapping ^{152}Eu and ^{56}Co measurements.

We took that curve, and just for the sake of the demonstration, manually removed the ^{56}Co lines which overlapped the ^{152}Eu ones, this way created two measurements

with disjoint regions of peaks. These two measurements cannot be used for a nonlinearity analysis.

In order to reduce the overall nonlinearity, the fitting algorithm applied a 'rotation' to the ^{56}Co measurement, and flattened out the whole curve significantly, giving an improper result. You should always avoid such situations, by adding another measurement or missing peaks to the nonlinearity analysis.

A possible solution would be to use a third measurement, which covers the middle region, while overlaps a bit with the first and the second measurements.

Problem No.3: Radiations not found

If nonlinearity analyzer is not able to find a particular peak, it is also possible that the matching library line has no the proper *radiation usage flag*. HyperLab uses a gamma line for nonlinearity purposes only if the "Use for nonlinearity" flag is assigned to it. See further details in section Nuclear data library management.

7. Detector efficiency analysis

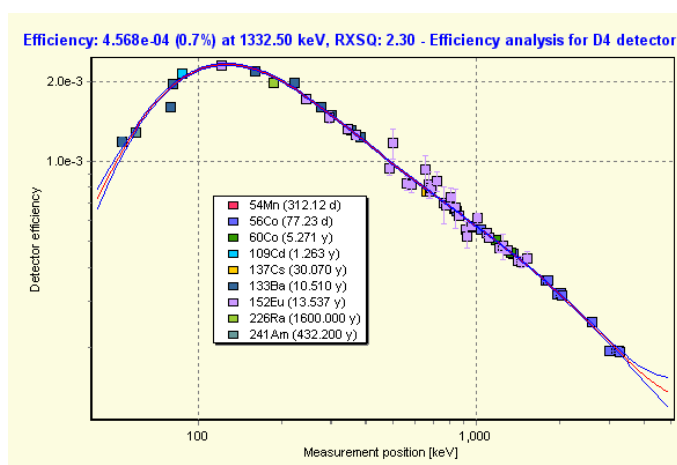
HyperLab is able to automatically construct absolute or relative full-energy detector efficiency functions (curves) from multiple measurements taken with multiple radioactive sources. The applied state-of-the-art techniques result in a single detector efficiency polynomial, and also its exactly computed uncertainty values throughout the used energy range. This provides significant advantage over HyperLab's competitors.

Efficiency curve

The semiconductor detectors' efficiency means a ratio between the number of photons arriving into the detector and the number of detected events resulting at the end of the measurement chain. As the probability of gamma photon detection changes rapidly with the energy of the photons, it is common to describe the logarithmic of the efficiency as a function of the logarithmic of the photon energy.

HyperLab also uses this $\log(\text{Eff})$ vs. $\log(E)$ fitting and displaying method in its *Detector efficiency analysis* module, as you can see in this figure.

The curve itself is depicted by a red line, its $\pm 1\sigma$ limit with blue lines, while the measured intensity points are either *not* normalized (if an absolute calibrated radioactive source is used) or normalized (in case of home-made sources).



The calculated detector efficiency may be used for generating special peak list reports, which contains peak areas and uncertainties with efficiency correction. Later versions of HyperLab will also contain nuclide identification based on the efficiency curve.

7.1. Algorithm of efficiency determination

Detector efficiency determination is easy with HyperLab's Efficiency module. Only several measurements and proper radioactive source entries are required, and a calibration curve may be constructed within a few minutes.

The algorithm of the efficiency determination is the following:

1. Determination of the matching gamma lines in the measurements. The list of gamma lines is generated from the matching radioactive sources' isomers or from manual assignment.
2. In case of absolutely calibrated sources, the belonging measurements will be used even if only one matching line is found in it. In case of relative measurements, at least two assigned lines are required. This is because a Y-shifting transformation will be applied to these points – in order to match the points from other measurements – and at least two points can only provide additional information about the shape of the curve.
3. One-step fit is performed on all identified points of all measurements with one common ortho-normalized polynomial, and optionally with several shifting parameters (one shifting parameter for each relative measurement). The shape of the polynomial describes the efficiency of the measurement system, while the shifting parameters normalize together the relative measurements together or to the absolute measurements, so that the common chi-squared is at the minimum.

7.2. Measurements required for the efficiency analysis

For nonlinearity determination, you need one or more multi-line measurements. The measurements should have the following properties:

- taken with the same measurement setup (same detector, ADC, energy range),
- taken roughly in the same time period (preferably within the same day, or within 1 week),
- their gamma lines of isotopes have *exact energy* values in HyperLab's database,
- the lines of the isotopes spread across your entire, regularly used *energy range*,
- the used decay gamma cascade does not show significant *true-coincidence summing* effect (either due to the structure of the nuclear transitions, or due to the appropriately large detector-source distance),
- every relative measurement has at least 2 proper gamma lines, and every absolute calibrated measurement has at least one proper gamma line.

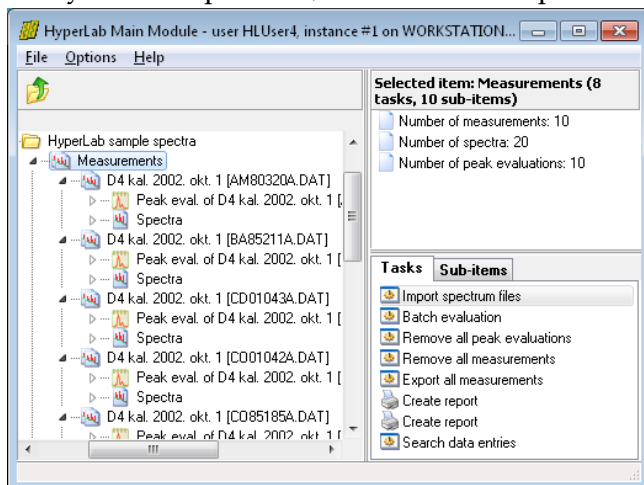
These are not stringent requirements, so the majority of usual calibration measurements – or even measurements acquired for material analysis – will be usable for efficiency determination. You can also use isotopes with a few problematic lines, as you will be able to individually remove the disturbing or overlapping lines from the efficiency curve.

7.3. Steps of efficiency determination

In order to determine the efficiency curve of a measurement system, first take some measurements with calibration sources (possibly with absolutely calibrated ones), and import them into your HyperLab database.

Our example will work with HyperLab's sample spectra belonging to a measurement setup with 70 keV - 3300 keV range. Please load the spectrum files into the database and also set their corresponding source values, as specified in section “Importing sample spectra”.

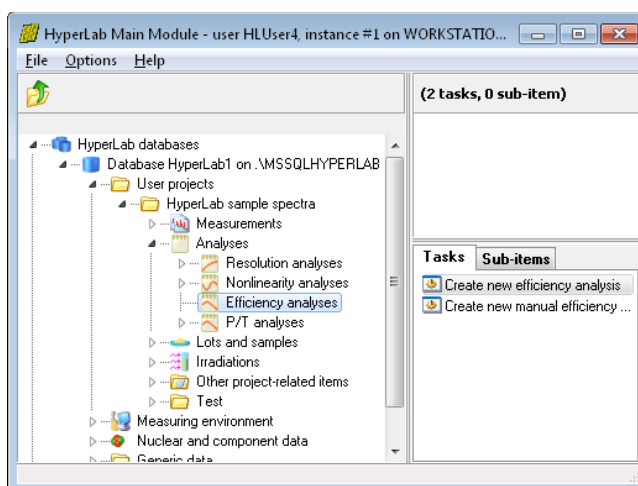
Perform a batch or individual evaluation on all measurements, and open a multi-line spectrum with the Peak evaluator. Check the FWHM calibration, and adjust the region fits, if necessary. Finally save the peak list, which will be input for the efficiency evaluation.



When all measurements are properly fitted, similar statistics will be displayed about them at the right side of the Main Module window as you can see in this picture. To ease the work of the spectroscopist, the same peak evaluations may be utilized for nonlinearity determination and for efficiency analysis.

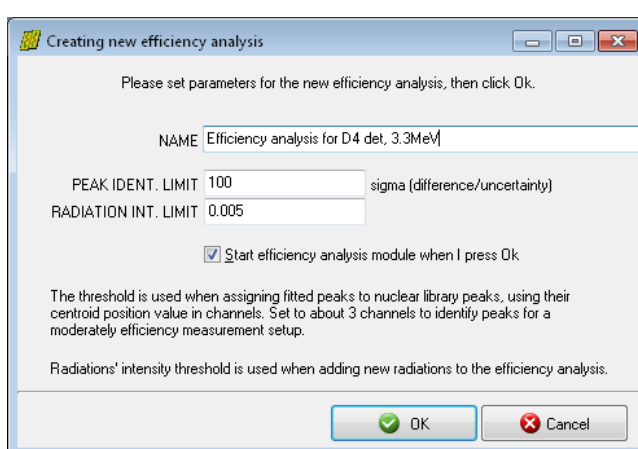
Open *Analyses* node under your project, then click on *Efficiency analyses* and select *Create new efficiency analysis* task.

A new window appears now, where basic parameters of efficiency fitting algorithm may be specified.



Here you can specify a descriptive name of the new efficiency analysis, and thresholds for the identification of peaks.

The *Peak identification limit* is used when peaklist peaks and nuclear library peaks are matched. If the difference between peak centroid and radiation's energy is below this Chi value (using the combined energy uncertainty value of the peak and gamma line), the peaks will be considered as matching.

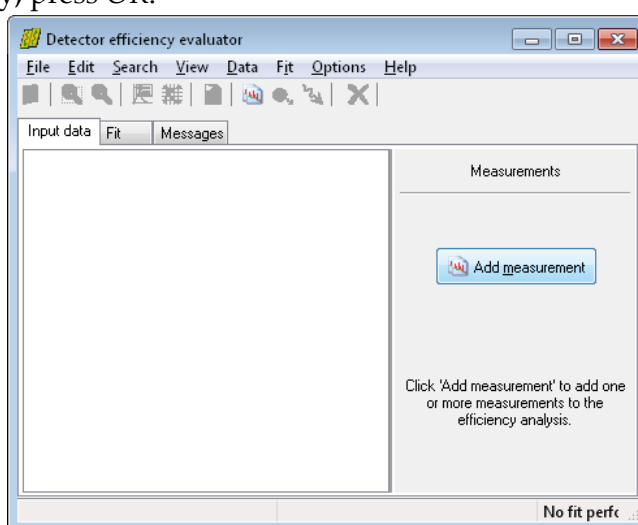


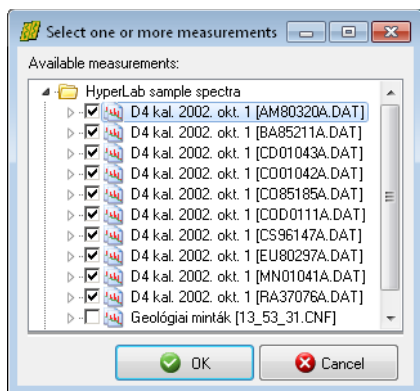
Its usual value is 100 Chi, which is appropriate even for cases when nonlinearity correction is not applied in the energy calibration, therefore huge differences may occur for peak positions. If you are using nonlinearity correction for all of your measurements used for the efficiency analysis, enter a value of 5.0 Chi here.

The *Radiation intensity limit* is used when radiations are loaded for a selected decay from the database. The 0.005 default value load the radiations where the intensity is greater than 0.5% of the decay's strongest line. When you are ready, press OK.

The *Detector efficiency evaluator* window appears now with the empty *Input data* sheet.

Click *Add measurement* button at the right. The *Measurement selector* window appears now.





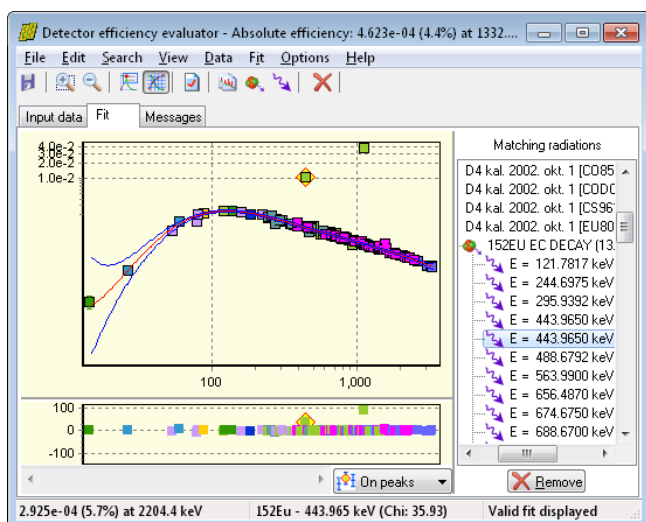
Select all of HyperLab's example measurements from the project.

When you click OK in the measurement selector window, HyperLab performs the steps as follows.

- Loads the peaks from the most recent peak evaluation of the measurement (this should be the *nonlinearity corrected* peaklist).
- Checks if a radioactive source is specified for the measurement. If found, loads its isomers and their radiations, as well as source activity details. Otherwise prompts the user for selecting the isotopes.
- Limits the radiations to those whose intensity is over the

preset intensity limit and which have a radiation usage flag, enabling the radiation for detector efficiency evaluation purposes.

- Matches the loaded radiations and their closest fitted peaks, by applying the preset matching limit.
- If at least one matching peak-radiation pair is found within a peak list (or 2 matching pairs for measurements taken with a home-made source), then the measurement may be used for efficiency evaluation.
- Checks if enough input data points exist for a polynomial fit. The number of data points must exceed the number of fitted parameters, i.e. the degree of the fitting polynomial plus one activity shifting parameter for each non-absolutely calibrated measurement.



If enough data points are identified, the fit will succeed and the tab Fit becomes active, displaying the fitted efficiency curve.

It will be an absolute efficiency curve if any of the matching measurements has an absolutely calibrated source, and it will be relative efficiency if no measurement has such source.

Now you can add other measurements to the fit one-by-one, or more at a time.

Eventually, a multi-measurement, multi-isotope efficiency curve may be easily constructed.

Improvement of the fit

If you check the resulting reduced Chi-squared (RXSQ=101) or the residual of the fit, it is immediately obvious that there is a problem with the fit.

Please be aware of the outlying 152Eu data points on the previous figure, which are far off from the efficiency curve. This is the 443keV line of 152Eu, and it is improper for calibration purposes because the level scheme contains two overlapping 443keV peaks. The similar problem exists with the 1112keV line of 152Eu EC decay and the 1109keV line of 152Eu β -decay.

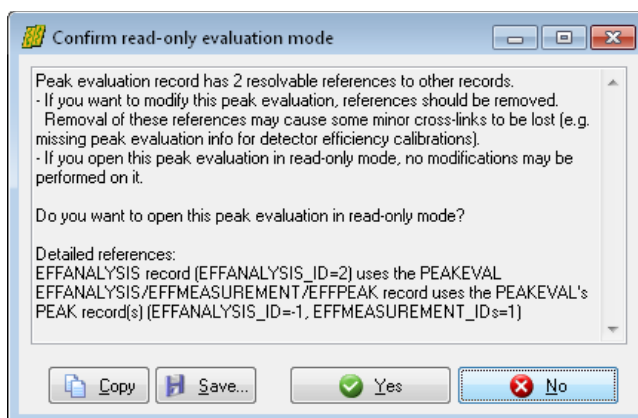
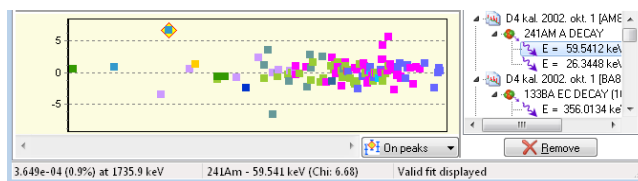
It is unavoidable to remove all of these disturbing lines. Select the first 443keV line by clicking on it (on the fit chart, or on the residual, or in the list of matching radiations), and then click *Remove* button, and repeat this for the other problematic line at 443keV. You can use the View/Sorting of radiations menu to display energy-sorted lines. Also repeat with 1112keV and 1109keV lines of 152Eu, and the notoriously weakly fitted 79keV line of 133Ba.

With those modifications, the RXSQ value goes down to around 3, which should also be improved.

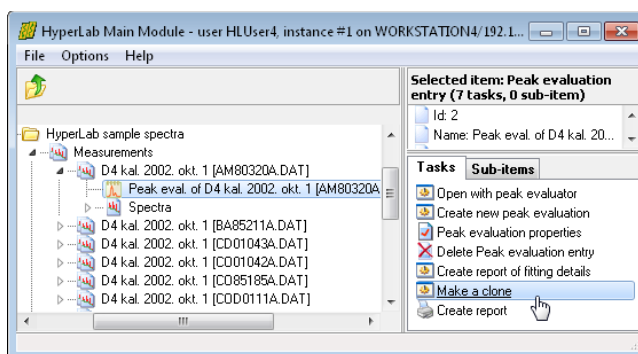
It is better to check the residuals now, to see which line exactly causes this problematic RXSQ. Click on the outlier point at 59keV. It is immediately displayed on the right that it belongs to 241Am.

In order to see the spectrum's details, save the efficiency fit, and open the 241Am peak evaluation.

If you have a warning about that this peak evaluation is already used in an analysis, therefore cannot be modified, then select No here.

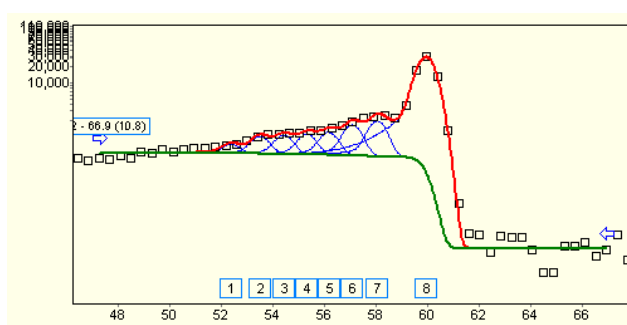


Now select the *Make a clone* task while the peak evaluation is selected, thus creating a new peak evaluation, which contains the same details as its original one, but editable. After cloning, a second peak evaluation appears on the left, at the database tree. For the sake of clearer further explanations, we changed its name to '2nd Peak evaluation'. Open this new evaluation, and check the problematic 59keV region.



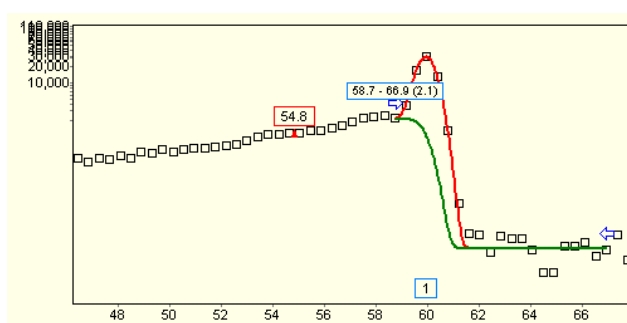
The problem may be evident at once: the automatic fit incorrectly included part of the background in the peak.

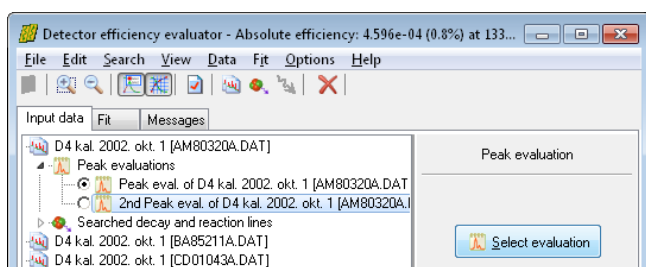
Move the left side of the region to right, by dragging the blue arrow to the base of the peak.



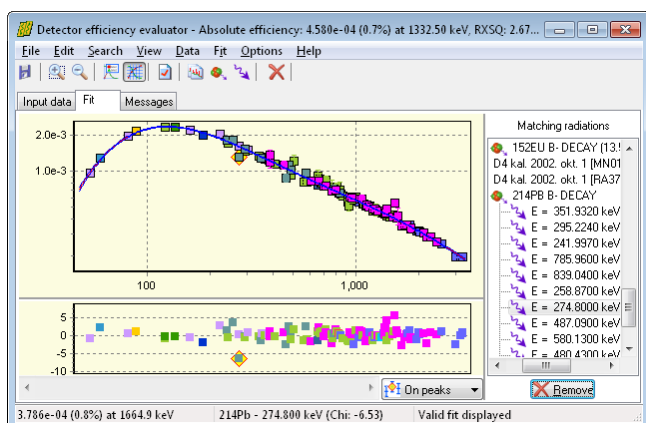
After the manual intervention, the area of the peak decreases significantly (change is over 5%, while its uncertainty was 1%). Now save this peak evaluation.

Open the efficiency analysis again.





On the input page, open the 241Am measurement, select the second peak evaluation node on the left, then click the 'Select evaluation' button on the right.



After removing two other low-energy lines, the figure shows the improved efficiency curve. It has RXSQ value of 2.7, which indicates a good fit – with only minimum user intervention.

If you have used the cloned peak evaluation, then the original one is possibly unused now, so you can delete it under the measurement entry.

7.4. Designating a proper efficiency curve as a default

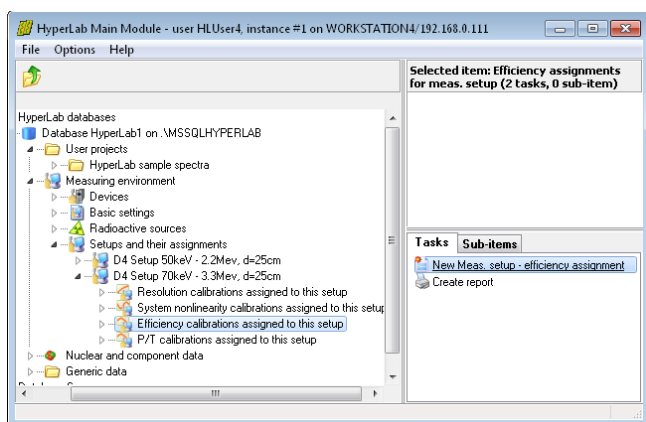
After a successfully construction of an efficiency curve, you should take one last administrative step: HyperLab should know that this curve is to be used as a default one. This can be done by assigning the efficiency analysis to the measurement setup where it belongs.

After this step, the efficiency of a measurement can be automatically determined, purely by its acquisition date and the measurement setup set up for the spectrum.

This is currently used by HyperLab for two purposes:

- nuclide identification is more convenient, as automatic loading of the matching efficiency curve is performed during spectrum deconvolution, and
- it is possible to generate an efficiency-corrected peak list (however, this is rarely used).

In order to assign an efficiency analysis to the measurement setup, please follow the instructions below.



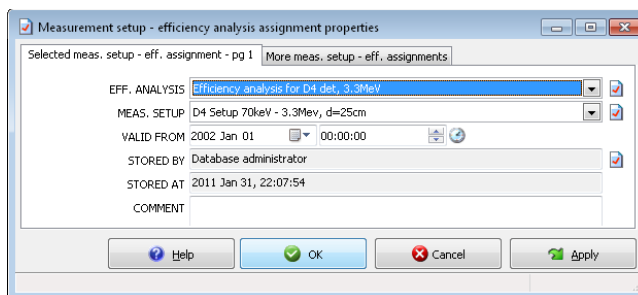
Open *Measuring environment* node in your database browser tree, then *Setups and their assignments*, finally the measurement setup where your efficiency curve is created. In our example, the measurement setup 'D4 Setup 70keV - 3.3Mev, d=25cm' was opened. After that entry, click *Efficiency calibrations assigned to this setup*, and then select the task at the right named 'New Meas. Setup – efficiency assignment'. A data entry window appears now.

Now you should select the efficiency analysis you have created.

Another important field is the *Valid from* entry, where you can define the starting date when your efficiency analysis should be used as a default.

Set it to the **date of the measurements** which have been used for the analysis.

In our example, we set this date to January 1st, 2002, to make sure that it will be automatically used for all measurements taken from the very first day of the year.

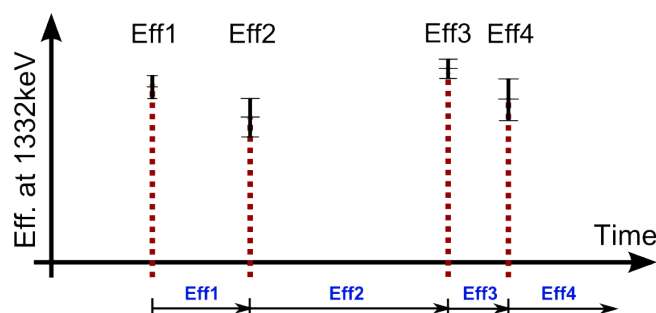


You should always register a successfully created analysis as default. This way a chain of efficiency curves will be created, each representing a time range of your measurement system, when that calibration was valid.

On this picture we depict a situation, when 4 efficiency analysis, Eff1 – Eff4 is assigned to the same measurement setup.

After the first assignment (Eff1), a default efficiency curve is existing in the system.

For example, when a measurement is loaded into peak evaluator, where the acquisition time is between the 2nd and the 3rd efficiency analysis (between Eff2 and Eff3), the efficiency curve Eff2 is automatically loaded, and the isotope identification will use it automatically.



7.5. Common problems during efficiency determination

Although efficiency determination is almost a trivial task with HyperLab, there may be common problems for the users. One such problem may arise with peak matching.

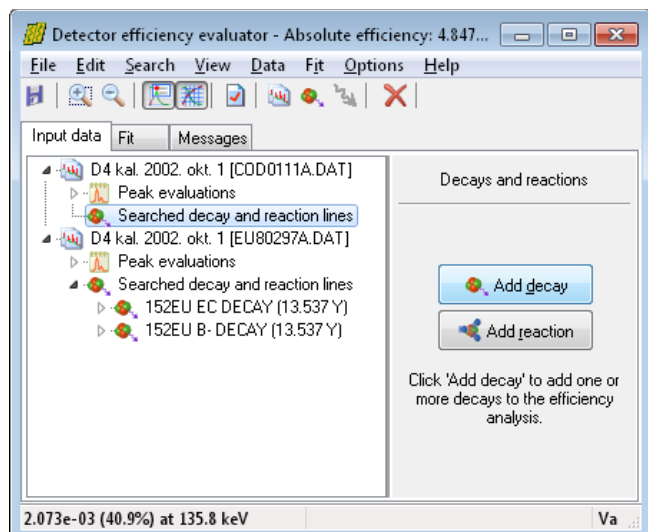
Problem No.1: Using the same measurements for nonlinearity and efficiency

If you want to determine the nonlinearity and the efficiency from the same measurement set, it is advisable to evaluate the measurements twice:

- evaluate the measurement with a purely linear energy calibration;
- create the nonlinearity calibration, and save it;
- load measurements into the peak evaluator again one by one, and assign the new nonlinearity to the energy calibration, then save a new peak list;
- load these new peak evaluations (which have now better energy calibrated peaks) into the efficiency evaluator.

Problem No.2: Decays not set

If you have selected a measurement, where the sample is not set to a radioactive source, HyperLab is not able to automatically assign decays and their radiations to the measurement. In this case the user should manually assign decays to the measurement.



To add decays, select *Input data* tab, then click on the *Searched decay lines* node under the measurement in question. If you open this node and no decay has been set, click *Add decay* on the right.

Select proper decay and click *OK*. HyperLab now loads the decay and its radiations, and performs a fit with the currently identified matching radiation-peak pairs.

Problem No.3: Radiations not found

When only a simple linear energy calibration is applied to a spectrum, large discrepancies may exist between the expected and observed peak energies. If this difference is greater than the identification threshold (100 chi by default), radiations will not be identified. Therefore it is very important to apply the precise energy calibration (together with nonlinearity) in the Peak evaluator for the calibration measurements.

To get detailed information about the peak matching, see radiations under the *Input data* tab, or select *File / General info* menu item. A detailed listing is provided here about the matching of all searched radiations.

Another reason for missing peak matching is the missing *radiation usage flag*. HyperLab uses a gamma line for efficiency determination purposes only if that radiation is equipped with "Use for efficiency" flag. See further details in section Nuclear data library management.

7.6. Using efficiency curve in third party applications

When an efficiency curve is constructed in HyperLab's detector efficiency analysis module, the fitted orthogonal polynomial is available from the *File / Generic info* menu item or in efficiency reports. A reported polynomial may be the following:

```
Eff = exp(
    -8.29004319788 -1.89376623371*T[1] -0.782232919684*T[2] -0.0814766195533*T[3]
    -0.684186229251*T[4] +0.0122364315926*T[5] +0.278512435801*T[6] )
X = -2.56318287167535 +0.393416534891053*loge(E_keV)
T[0] = 1.0
T[1] = X -0.265941444781564
T[2] = (X -0.114813912833466)*T[1] -0.217642251256021*T[0]
T[3] = (X +0.123855849579396)*T[2] -0.233867482021834*T[1]
T[4] = (X +0.070373668815714)*T[3] -0.413775078142546*T[2]
T[5] = (X -0.132282651671386)*T[4] -0.124487482871051*T[3]
T[6] = (X +0.176131058246229)*T[5] -0.330089517919545*T[4]
```


The corresponding high-precision calculation function in C language:

```
double Eff( double E_keV ) {
    double T[7], X = -2.56318287167535 +0.393416534891053 * log( E_keV );
    T[0] = 1.0;
    T[1] = X -0.265941444781564;
    T[2] = (X -0.114813912833466)*T[1] -0.217642251256021*T[0];
    T[3] = (X +0.123855849579396)*T[2] -0.233867482021834*T[1];
    T[4] = (X +0.070373668815714)*T[3] -0.413775078142546*T[2];
    T[5] = (X -0.132282651671386)*T[4] -0.124487482871051*T[3];
    T[6] = (X +0.176131058246229)*T[5] -0.330089517919545*T[4];
    double Eff = exp(
        -8.29004319788 -1.89376623371*T[1] -0.782232919684*T[2]-0.0814766195533*T[3]
        -0.684186229251*T[4] +0.0122364315926*T[5] +0.278512435801*T[6] );
    return Eff;
}
```

The formula above is also reported to the user as a regular polynomial, which is the more usual description of the log Eff vs. log Energy dependency. See the formula at the *File / General info* menu.

A possible transcription in C:

```
double Eff_regular( double E_keV )
{
    double LogE = log(E_keV), LogE2=LogE*LogE, LogE4=LogE2*LogE2;
    double LogEff =
        30.6835240174 -46.5504384031*LogE +21.9649579373*LogE2
        -5.14575805865*LogE2*LogE +0.640226601624*LogE4
        -0.0406273018462*LogE4*LogE +0.00103266687194*LogE4*LogE2;
    return exp( LogEff );
}
```

Please note that due to the inherent numerical instability of regular polynomials, you must preserve as many significant figures in the coefficients as you can, otherwise imprecise values will be computed. At least 10-12 digits are strongly recommended.

An equivalent, and a bit numerically more stable calculation method is the following:

```
double Eff_regular_stable( double E_keV )
{
    double LogE = log(E_keV);
    double LogEff =
        30.6835240174
        +LogE*(-46.5504384031
        +LogE*(+21.9649579373
        +LogE*(-5.14575805865
        +LogE*(+0.640226601624
        +LogE*(-0.0406273018462
        +LogE*(+0.00103266687194))))));
    return exp( LogEff );
}
```

8. Spectrum peak evaluator

Spectrum peak evaluator plays a key role in HyperLab, as this module makes it possible to evaluate your spectra in a visually rich graphical user interface. After you performed a fully automatic spectrum deconvolution, you can quickly revise the fits visually, and adjust the problematic regions to your needs with our convenient spectrum manipulation tools.

Peak fitting algorithm

Predecessor of HyperLab's state-of-the-art algorithm was HYPERMET, which was developed for mainframes by the Naval Research Laboratory in the 1970's (see article in NRL Memorandum Report 3198, January 1976; G.W. Phillips and K.W. Marlow: Program HYPERMET for Automatic Analysis of Gamma-Ray Spectra from Germanium Detectors). A later variant was Hypermet-PC, which was a DOS-based clone for PCs.

HyperLab's automatic deconvolution is completely rewritten from scratch, retaining the original concepts and eliminating many constraints, limitations and faulty algorithms.

8.1. Control flow of the deconvolution

The new deconvolution algorithm comprises several fine-tuned steps:

- A list of suspected peaks created, based on the FWHM calibration. This is done by applying a simple, rectangular, convolution-type peak search function.
- Determination of region bounds follows. Regions are consecutive channel ranges, with one or more peaks, where the measured background may be described by the sum of HyperLab's various background functions. Regions are determined to be wide enough for the safe background function determination, but close enough to the peak to prevent unnecessary overlapping of background with peaks.
- A spectrum deconvolution is performed for the region. Various parameters are fitted in this step, in order to find the best match between the model function and the measured counts. The measure of the matching utilizes variances of counts – and possibly the Westphal-corrected variances in case of Dual LFC measurements. This way the fitted areas are corrected properly for count losses.
- If the fit is not satisfactory, an iterative refinement process is started, when new peaks may be added, removed, or the region bounds extended or collapsed. This flexible automatic self-adjustment makes HyperLab an outstanding deconvolution tool.
- After a best matching deconvolution is found, the final steps follow: elimination of unnecessary fitted parameters and calculation of peak areas together with their uncertainties.
- When a region deconvolution is finished, the next region is taken until the end of the spectrum.

After spectrum fitting, a peak list is presented to the user, together with graphical representation of the fitted regions.

8.2. Model functions of peak fitting

HyperLab's several model functions together describe the measured counts in gamma spectra taken with semiconductor detectors. These model functions are originated from their simplified HYPERMET variants, but re-implemented with up-to-date techniques.

Model functions may be either peak type functions – Gaussian, Left Skew and Right Skew –, or background type functions: Polynomial, Step and Tail. Peak functions are summed up, resulting in the peak areas, which are reported to the spectroscopist. The basic idea behind the deconvolution is a nonlinear fitting algorithm, which adjust free parameters between well-defined limits, thus achieving a good agreement between the measured counts and the sum of all background and all peak functions.

The following sections will describe the individual peak function in greater detail.

8.2.1. Gaussian peak function

The Gaussian component contains the majority of peak counts. This component arises from the statistical noise which broadens the sharp line response of an ideal detector.

The fitted parameters for Gaussians are the Position, the Amplitude and the Width.

Its counts may be calculated by the following formula at channel x :

$$\text{Gaussian} = \text{Ampl} \cdot \exp\left(-\frac{(x - \text{Pos})^2}{\text{Width}^2}\right)$$

where

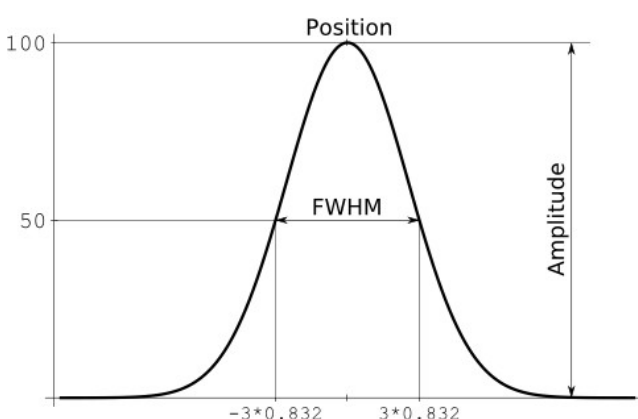
Ampl: Amplitude of peak

Pos: Position of the centroid

Width: Peak width parameter, so that $\text{FWHM} = 2 \cdot \text{Width} \cdot \sqrt{\log(2)}$ or $\text{Width} = \text{FWHM}/1.66$

The picture shows a Gaussian with $\text{Position}=0$, $\text{Width}=3$ and $\text{Amplitude}=100$. In this case FWHM is $6 \cdot \sqrt{\log(2)}$.

The X axis depicts channel positions in a spectrum region (zero selected for the peak centroid just for convenient display), while the Y axis shows count values.

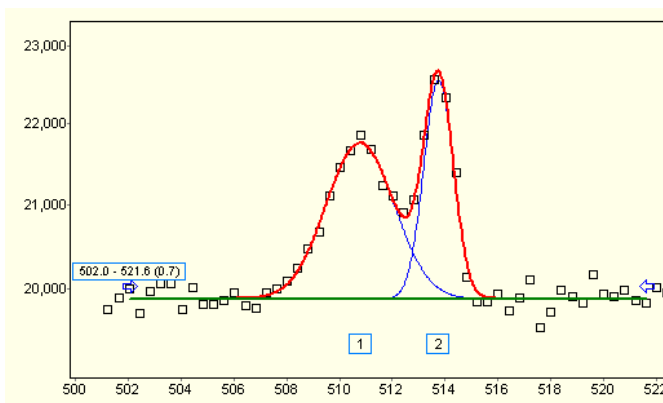


Peak width determination variants

Users in HyperLab may choose from two different approaches when determining the width of the Gaussians in a region.

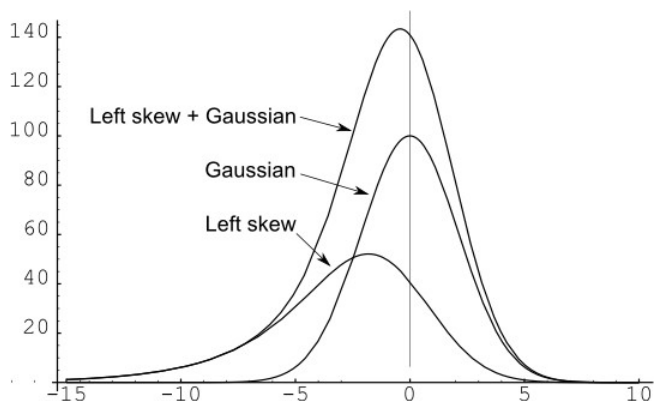
The first is the *Common peak width method*, which is based on gamma spectroscopy heuristics, as it fits one common peak width for each peak within a region. This model is able to describe the majority of the spectrum regions.

There are cases, however, when the *Variable peak width method* is required: this fits peak width for each Gaussian individually. A typical example for this case is the extremely broadening 511keV annihilation peak, where valuable peaks of various radioisotopes should be separated automatically from the annihilation peak. See "Peak evaluation algorithm settings window" for further details.



8.2.2. Left skew peak function

Left skew is a peak function, that is, its integral over the region will be summed to the peak area. It is introduced because an electron energy shifting occurs regularly towards the lower energies, due to the incomplete charge collection in the detector crystal.



Because it is originated from a convolution of a Gaussian and an exponential, which is allowed to increase until the Gaussian's centroid, it is an asymmetric function. Therefore when the left skew is added to a Gaussian peak, it causes slight increase at the low energy side of the peak.

The fitted parameters for Left skew are the Left Skew Amplitude (relative to the Gaussian's amplitude), and the Left Skew Slope. The width of the left skew is not fitted, but assumed to be always equal to the width of the Gaussian. The picture shows a left skew with Slope=1 and relative Amplitude=0.25. Please note that skew may take part significantly in the total peak area.

Left skew's counts may be calculated by the following formula at channel x :

$$LeftSkew = Ampl \cdot \frac{\sqrt{\pi}}{2} \cdot Width \cdot LSAmpl \cdot \exp\left(\left[\frac{Width}{2 \cdot LSSlope}\right]^2 + \frac{x - Pos}{LSSlope}\right) \cdot \operatorname{erfc}\left(\frac{Width}{2 \cdot LSSlope} + \frac{x - Pos}{Width}\right)$$

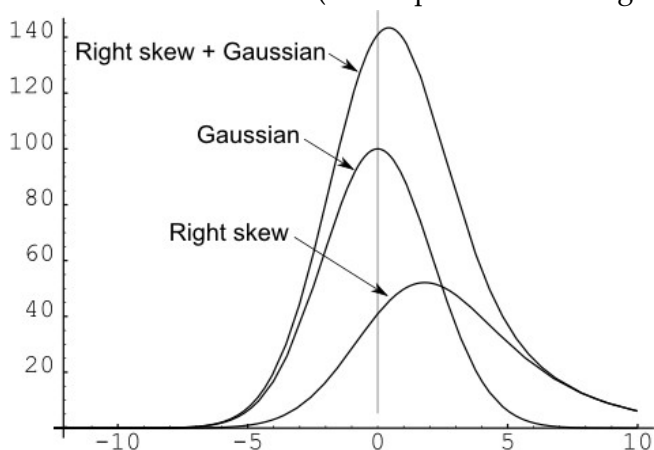
where

- LSAmp*: Left Skew Amplitude relative to that of Gaussian (may vary from 0.0 to 0.75)
- LSSlope*: Left Skew Slope (0.3 – 2.0)
- Ampl*: Amplitude of Gaussian
- Pos*: Position of the Gaussian centroid
- Width*: Gaussian width ($Width = FWHM/1.66$)

and erfc is the standard complementary error function.

8.2.3. Right skew peak function

Right skew is the third peak function, and its integral will also be summed up to the peak area. Right skew is not included by HyperLab's predecessors, but it is present in HyperLab to allow better deconvolution. It may be of great importance, because skewness on the high energy side of the peak quite frequently occurs in practice (e.g. in short time activation analysis) due to pile-up effects. Right skew is very similar to Left skew which is at the low-energy side of a Gaussian, but it is mirrored to that (its flat part is on the high-energy side).



Because it is originated from a convolution of a Gaussian and an exponential, which decreases starting from the Gaussian's centroid, it is an asymmetric function. Therefore when the right skew is added to a Gaussian peak, it causes slight increase at the high energy side of the peak.

The fitted parameters for Right skew are the Right Skew Amplitude (relative to the Gaussian's amplitude), and the Right Skew Slope. The width of the right skew is not fitted, but assumed to be always equal to the width of the Gaussian. The picture shows a right skew with Slope=1 and relative Amplitude=0.25.

Right skew's counts may be calculated by the following formula at channel x :

$$RightSkew = Ampl \cdot \frac{\sqrt{\pi}}{2} \cdot Width \cdot RSAmpl \cdot \exp\left(\left[\frac{Width}{2 \cdot RSSlope}\right]^2 - \frac{x - Pos}{RSSlope}\right) \cdot \operatorname{erfc}\left(\frac{Width}{2 \cdot RSSlope} - \frac{x - Pos}{Width}\right)$$

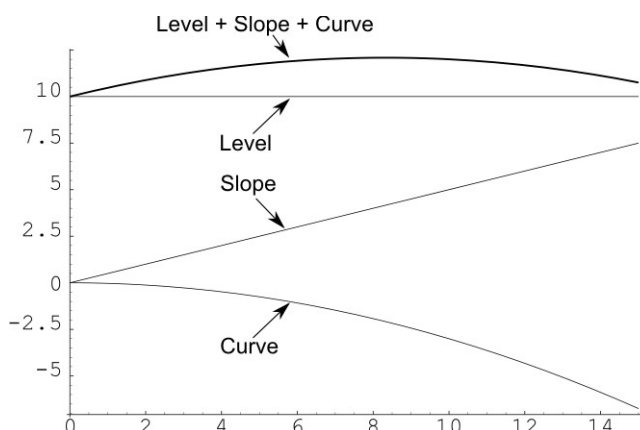
where

RSAmpl: Right Skew Amplitude relative to that of Gaussian (may vary from 0.0 to 0.75)
RSSlope: Right Skew Slope (0.3 – 2.0)
Ampl: Amplitude of Gaussian
Pos: Position of the Gaussian centroid
Width: Gaussian width ($Width = FWHM/1.66$),
 and *erfc* is the standard complementary error function.

8.2.4. Polynomial background function

Polynomial background component is able to characterize the continuous, slowly changing background under peaks.

It is implemented as a second order polynomial in the region, so constant, slanting or curved (parabolic) background may be modeled with it, freely combining its counterparts. As a background function, its area will *not* be summed up to the peak area. It may have at most three fitted parameters: Level, Slope and Curvature. The picture shows a sample polynomial background with Level=10, Slope=0.5, Curve=-0.03 parameters.



Counts from the polynomial background may be calculated by the following formula at channel *RegionPos*:

$$PolyBkg = Level + Slope \cdot RegionPos + Curve \cdot RegionPos^2$$

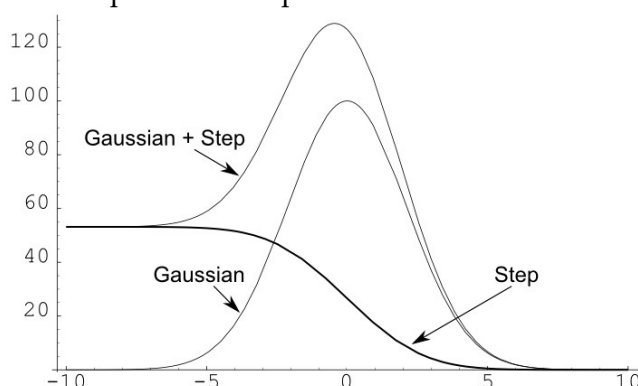
Where

RegionPos: Channel position within the fitted region (first channel of the region is 0)
Level: Constant background level
Slope: Background slope (may be positive or negative)
Curve: Background curvature (may be positive or negative)

8.2.5. Step background function

HyperLab also fits regions with sharp background steps under the peaks.

This stepped background accounts for a Compton edge. Steps are fitted by one characteristic parameter, the Step Amplitude, which is relative to the amplitude of the Gaussian. The picture shows a step with relative Amplitude=0.10.



Step's counts may be calculated by the following formula at channel *x*:

$$Step = Ampl \cdot \frac{\sqrt{\pi}}{2} \cdot Width \cdot STAmpl \cdot erfc\left(\frac{x}{Width}\right)$$

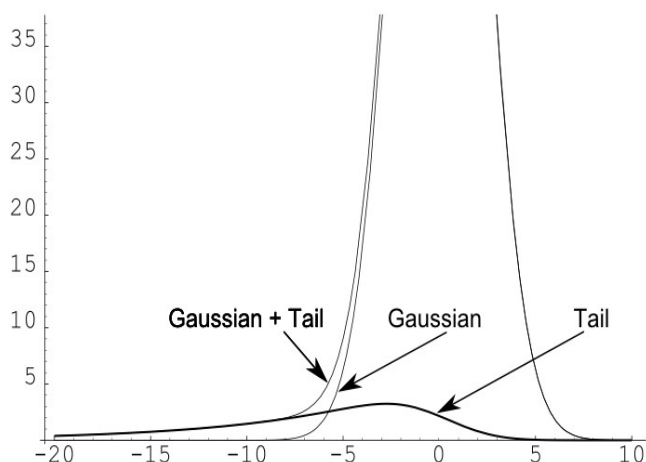
where

STAmpl: Step Amplitude relative to that of Gaussian

Ampl: Amplitude of Gaussian
Width: Gaussian width ($Width = FWHM/1.66$),
 and *erfc* is the standard complementary error function.

8.2.6. Tail background function

According to the original HYPERMET concept, a slowly decreasing exponential background tailing component may also be used under the low energy side of the peaks, in order to compensate detector surface effects.



Nowadays, however, this phenomenon seems to be less significant with the most common detectors, therefore when you perform a peak evaluation with “Default settings for moderate count rate, regular peaks” configuration, tail will be *disabled*. As tail also descends from a convolution of an exponential and a Gaussian, it is very similar to Left skew, but has much less intensity and greater slope. Important difference, however is that the tail is component of the background, while skew is a part of the peak.

Therefore counts under the skew is added to the peak area, while the area under the tail only contributes to the sum of background and peak functions, which helps the nonlinear fitter to match the measured counts. The picture shows the case of Tail Amplitude=0.01 and Tail Slope=2.5 parameters.

Tail counts may be calculated by the following formula at channel x :

$$Tail = Ampl \cdot \frac{\sqrt{\pi}}{2} \cdot Width \cdot TLAmp \cdot \exp\left(\left[\frac{Width}{2 \cdot TLSlope}\right]^2 + \frac{x - Pos}{TLSlope}\right) \cdot erfc\left(\frac{Width}{2 \cdot TLSlope} + \frac{x - Pos}{Width}\right)$$

where

TLAmp: Tail Amplitude relative to that of Gaussian (may vary from 0 to 0.01)
TLSlope: Tail Slope (2.5 – 50)
Ampl: Amplitude of Gaussian
Pos: Position of the Gaussian centroid
Width: Gaussian width ($Width = FWHM/1.66$),

and *erfc* is the standard complementary error function.

Note: If you observe significant scattering of Chi values in the peak fitting residual under the majority of the singlet peaks, and this may not be resolved by adding new peaks, it is possible that the background tail component should be enabled. This may be done either by manually enabling the component in the *Peak evaluation algorithm settings window*, or selecting another algorithm setting, where tail has been enabled previously. This is, however, may designate that your measurement set-up is improperly set or became noisy.

8.3. Starting the spectrum peak evaluator

A short evaluation introduction is provided in the *Quick Start Guide for Main Module* for the novice users. The following sections will detail the process of the peak evaluation.

The spectrum peak evaluator may be started in two ways:

- Creating a new peak evaluation entry in the database, which does not contain any fitted peaks. In this case only the measured counts appear in the peak evaluator window.

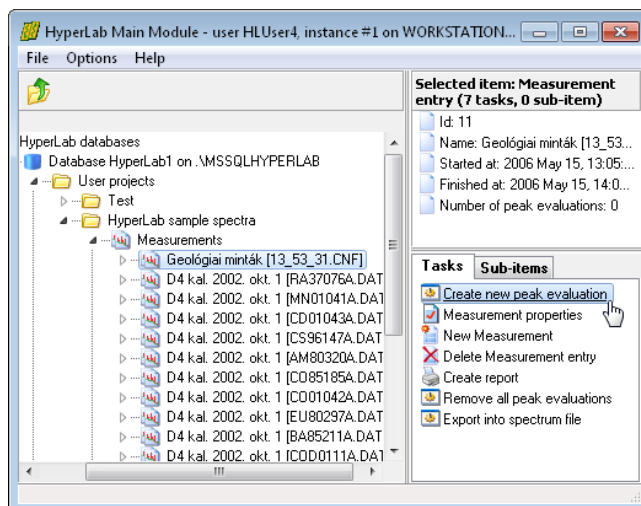
- Loading and possibly modifying a previously created peak evaluation entry, with all of its fitted and stored region and peak parameters. All previously fitted peaks are immediately displayed in this case.

8.3.1. Creating a new evaluation

To create a new peak evaluation entry and start the Peak evaluator, select your measurement in the database browser tree, then click task *Create new peak evaluation* in the Tasks window.

Alternatively, you can hit the *Enter* key, after you selected the measurement node, as *Enter* key will always start the currently selected task.

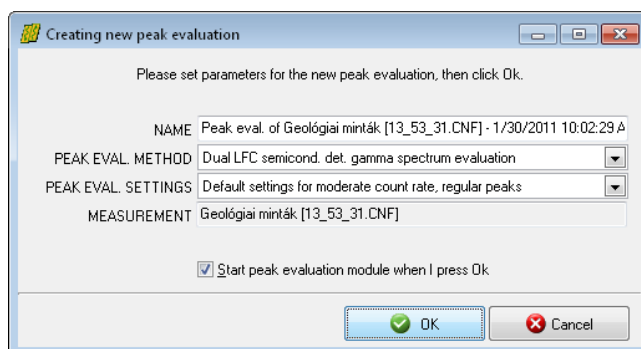
A window appears now, which lets you create a new peak evaluation entry in the database.



The *Peak evaluation method* list should not be modified, as this is set according to the type of spectrum entries belonging to the measurement.

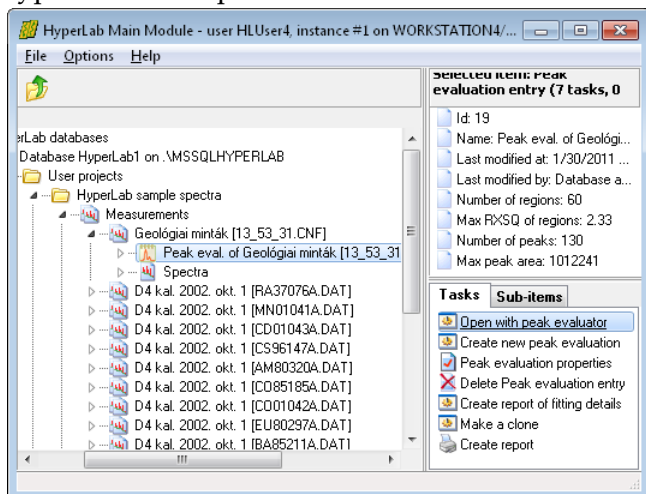
The *Peak evaluation settings* comprises fine-tuning options for the peak evaluator's algorithm. You can leave defaults in most cases, but if you regularly perform the evaluation with non-default parameters (e.g. with enabled *Tail* peak component), you may select different options here.

See more details in sections “Peak evaluation algorithm settings window” and “Model functions of peak fitting”.



8.3.2. Loading a previously created peak evaluation

HyperLab stores peak evaluation details in its databases, together with the spectrum entries.



To load and possibly modify a previously created peak evaluation entry, open the node of the proper measurement by clicking on the [+] sign, and select the proper peak evaluation node beneath it.

Now the peak evaluator window appears. It will contain spectrum counts, as well as all previously fitted regions and peaks.

8.3.3. Automatically loaded entries

After creating a new evaluation, or selecting an existing one, the spectrum peak evaluator window appears. HyperLab now loads all necessary entries of the peak evaluation from the database:

- the measurement entry;
- its spectrum entries (e.g. a *Normal* and an *LFC-corrected* spectrum part in case of Dual LFC measurements);
- latest FWHM calibration for the spectrum entries;
- latest energy calibration for the spectrum entries, together with nonlinearity calibration, if that is selected by the user on the Energy calibration editor window;
- detector efficiency curve for the measurement setup, if existing. This may be used for efficiency-corrected peak area calculations in the output reports.

Usage of latest FWHM and energy calibrations

Although you can save several independent peak evaluations for a specific measurement, when you re-load them later, the latest FWHM and energy calibration will be loaded. If you have modified these calibrations in the meantime, saving of the peak list may result in slightly different peak positions or peak fits. This way the exact reproduction of previous fitting results also requires the restoring of previous calibrations.

Ensuring automatic loading of the efficiency curve

HyperLab is able to automatically determine which detector efficiency curve belongs to a particular measurement. If such an efficiency curve is found, it will be automatically loaded by the peak evaluator, and efficiency corrected peak list reports may be generated.

To check if the efficiency analysis is successfully loaded, change to the *Messages* panel after you started the peak evaluator, and search for a message about the status of the efficiency loading. In order to ensure the automatic determination of the efficiency curve belonging to a specific measurement, you must perform the following two steps before starting the peak evaluator.

- Create a quality efficiency curve, where the relative uncertainty of the full-energy absolute detector efficiency is around the precision of your calibrated radioactive sources. For example, if you have taken measurements of absolutely calibrated radioactive sources with 1-2% activity uncertainty, then the efficiency value calculated

from the efficiency curve is also expected to have 1-2% uncertainty. Store this efficiency analysis into your database.

- Assign the efficiency analysis to the measurement setup entry where the measurements were taken. Do not forget to set the validity start date. HyperLab will automatically use this efficiency calibration for all the measurements, which were taken after this validity date (and before the validity start date of the next assigned efficiency curve). When multiple efficiency curves are assigned to the same measurement setup, their validity start dates will determine the one to be applied for a specific acquisition.

Creating reports with efficiency corrected peak areas

Saving of efficiency-corrected peak areas may be achieved in several ways:

- Select the File / Create report menu item, and select a report template where the description of the report shows “efficiency correction”.
- Select File / Export to CSV file menu item, and you will get a report which can be immediately loaded into a spreadsheet application.

The reports will contain the efficiency value at the energy of the peak centroid, relative uncertainty of the efficiency, as well as the efficiency corrected peak area together with its uncertainty (combined from the uncertainty of the peak area and the uncertainty of the efficiency curve at the centroid).

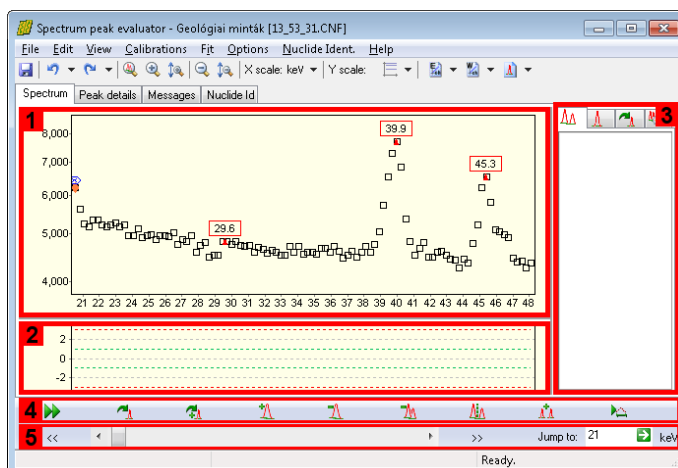
8.4. Basic parts of the evaluator window

The peak evaluator window is comprised of several re-sizable parts.

The center of the window is occupied by the **spectrum window** [1] and the **residual window** [2]. The residual window displays the difference between the measured counts and the fitted peak curves.

A **fit detail panel** [3] is placed on the right, while a **fit fine tuning toolbar** [4] and a **navigating toolbar** [5] is at the bottom. A **main toolbar** [6] is at the top of the window.

List of fitted peaks is displayed under the *Peak details* tab.

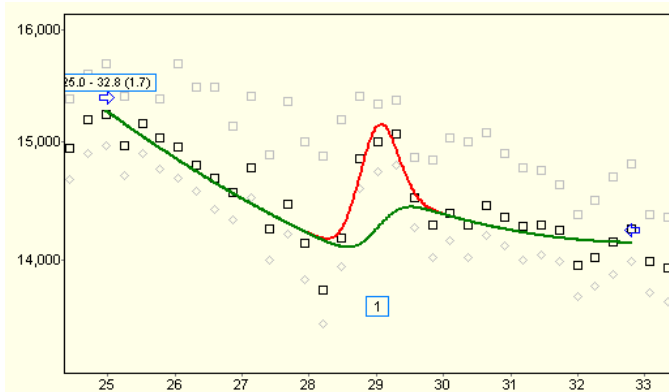


8.4.1. Elements of the spectrum window

Spectrum window displays spectrum and peak evaluation information graphically.

This section describes *static* display elements as well as *dynamic* display elements, which also provide controls for quick fit manipulation.

Spectrum window is basically an X-Y chart, which depicts spectrum details on a counts versus energy scale.



Horizontal axis of spectrum chart

Unit of horizontal axis of the spectrum chart may be either *channel* or *keV*, while its scale is always linear. Toggling between these units may be accomplished in several ways:

- Clicking on the “*keV*” or “*ch*” label on the navigating toolbar.
- Selecting the proper unit from the main toolbar's “*X unit*” drop-down list.
- Selecting *View / Energy scale for positions* menu.
- Pressing *Ctrl-N* keys simultaneously.

Vertical axis of spectrum chart

The unit of the vertical axis of the spectrum chart is always *count*, but its scale may be either *linear* or *logarithmic*. Toggling between these scaling modes may be initiated in several ways:

- Selecting the proper scaling from the main toolbar's “*Y scale*” drop-down list.
- Selecting *View / Logarithmic scale for counts* menu.
- Pressing *Ctrl-L* keys simultaneously.

Other axis settings (grids, tick marks etc.) temporarily may be set by selecting *Edit / Edit fit chart* menu, and selecting *Chart / Axis* tabs, then *Left Axis* item from the list. This may be helpful e.g. when special screen capture is needed.

Spectrum counts

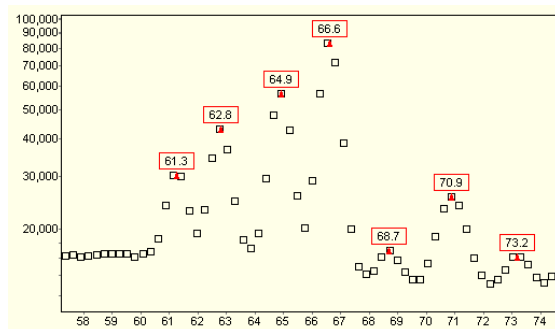
At most three kinds of counts may be displayed in the spectrum window:

- *Counts to be fitted* as black squares. These are either uncorrected counts (in case of regular gamma spectra), or loss-corrected counts (in case of some Loss Free Counting method), created by some kind of compensation electronics.
- *Uncorrected variances* as gray diamonds, as found in the original spectrum file. These values hold information about uncertainties for each channel of the measured counts. For regular gamma spectra, the values are almost identical with the counts to be fitted (only a small correction is applied for very low counts). In case of Loss Free Counting methods, these are from the Dual LFC spectra's uncorrected half (e.g. for Canberra's spectra), or from a special compensated spectrum half (e.g. “ERR” spectrum half for Ortec's ERR-ZDT spectra).
- *Count variances* as gray squares. These values are computed by HyperLab, possibly by applying Westphal-correction on original variance values. This is required in some cases because the loss-corrected counts have greater statistical variance than the non-corrected ones. As HyperLab fits the corrected counts by its peak functions, proper uncertainties are required during the fit.

For everyday purposes, it is necessary only to display the counts to be fitted, and the other counts are just for checking the details when you are interested in finer details. To switch off displaying the count variances, select *View / Chart Details* menu, then remove check marks beside *Count variances* and *Uncorrected count variances* menu items.

Suspected peaks

Please note the red triangles in the spectrum window: these are the **suspected peaks**, whose position is determined by the help of the current FWHM calibration before the deconvolution. The peak search is performed by a zero-area square wave convolution. The final spectrum deconvolution will use these suspected peaks as an initial estimation of peak positions, when the fit model is determined.



The list of suspected peaks is always re-generated when you change the FWHM calibration. The suspected peaks are replaced by the fitted peaks after a spectrum deconvolution. Sometimes the suspected peaks remain in the spectrum window, even after a whole-spectrum automatic fit. This is because sometimes the peak search algorithm finds spurious peaks, which are not replaced with real fitted peaks by the peak deconvolution algorithm.

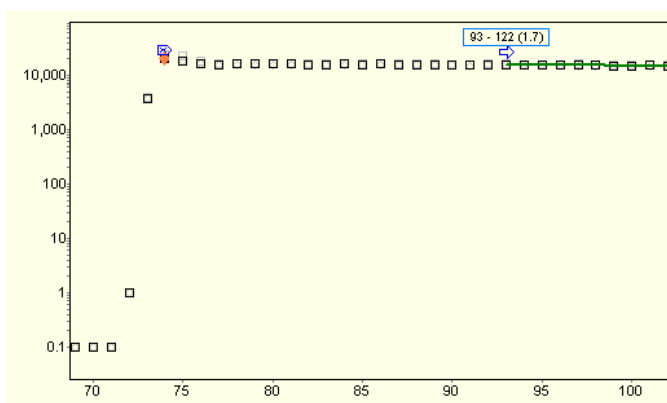
Left and right fitting threshold markers

When a spectrum is loaded into the spectrum peak evaluator, a left and a right channel threshold value is detected automatically.

The limits are designated by a framed blue 'X' pointing rightwards and leftwards.

The peak search algorithm will locate suspected peaks only between these outer values. In most cases, this automatic threshold determination works well, but a manual adjustment may be necessary in some very special cases.

If adjustment is needed, just click on the blue sign and drag it to its new position.



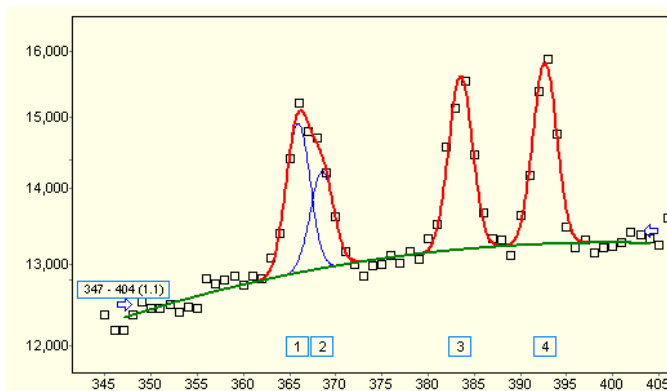
Plot of deconvoluted regions

After spectrum deconvolution is performed, fitted regions will be displayed.

The sum of background functions (2nd order polynomial background, step, tail) is drawn by green, while the sum of peak functions (Gaussian, left and right skew) and the background will be plotted by red color. The peak functions of the individual peaks are plotted by blue lines, in order to depict finer details within closely joined multiplets. *Peak labels* are displayed under the peaks with their serial numbers, while *region labels* contain basic region information

(region bounds and the reduced Chi-squared) at the beginning of the regions. These displayed items may also be configured through *View / Chart details* menu.

If you want to quickly adjust the plot to a specific fitted region, just *left-click* over it, and the spectrum chart will be immediately updated, zooming to the clicked region.



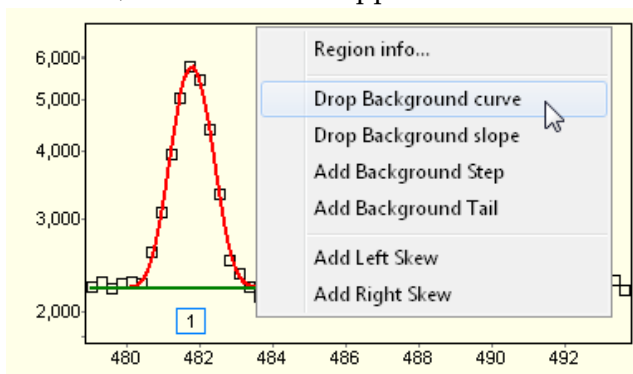
Left and right region bound marker arrows

At the beginning and the end of the plot of regions two *blue arrows* are displayed, which point towards the center of the region. If a region bound adjustment is needed, simply click and drag the proper arrow to its new place. After releasing the mouse button, an automatic fit takes place with the new bounds, and the new fit will be displayed.

Context-sensitive menu for fitted regions

When you right-click over a fitted region by the mouse, a context menu appears.

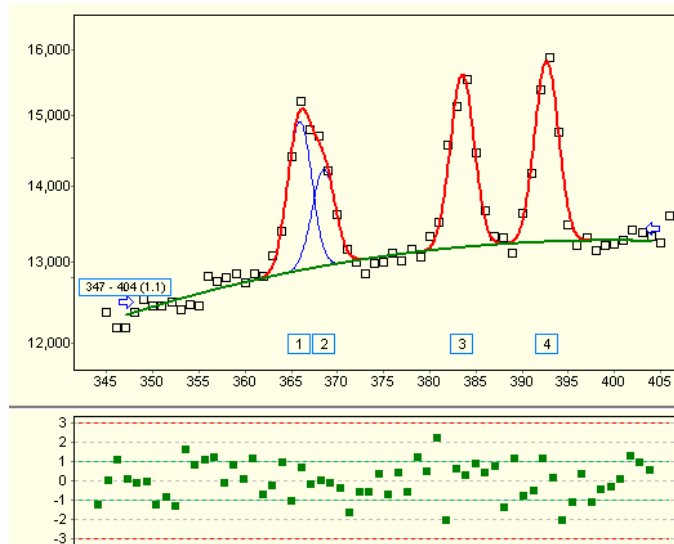
Its *Region info* menu item provides you a quick access to the details of the region fit. The other menu items allow a one-click fitting model manipulation, as the background and the peak skew fitting function components may be eliminated with them. This tool may lead to a trial-and-error refinement method, but it can be surprisingly effective on typical misfit situations.



If the region fit becomes significantly worse after dropping a component, just press *Undo* button on the main toolbar, and the previous fitting model will be immediately restored.

8.4.2. Elements of the residual window

The residual window displays the difference between the measured counts and the de-convoluted peak curves. It is placed beneath the spectrum window, and its X axis is always adjusted according to that.



The chart shows the difference between the measured and the fitted value for each measured value with *filled green squares*, in standard deviation units. If this value is positive, then the measured count value is greater than its matching fitted count.

Due to the statistical nature of the measured counts, we never expect a perfect matching between measured and fitted counts. *Chi* value is the ideal measure of the difference, because it takes into consideration the statistical variance of each measured count value, thus shows the significance of the difference, instead of its absolute value.

On the chart, the $\text{Chi}=1$ limit is designated by a green dashed line, while a red dashed line shows the $\text{Chi}=3$ limit.

As a rule of thumb, if the absolute value of the difference is less than 1, it is considered not significant (no further improvement is required). On the other hand, if it is greater than 3, it is highly improbable that the difference is purely from the statistical scattering of counts, and closer inspection is needed in the vicinity of that channel.

The normalized sum of squared Chi values gives the *Normalized Chi-Squared* value (RXSQ, Reduced Chi-squared, χ^2), which describes the quality of the fit for a whole region, and displayed in the region label at the first channel of the region. If RXSQ is significantly higher

than 1.0, a manual refinement of the region fit is advisable.

8.4.3. Elements of the fit detail panel

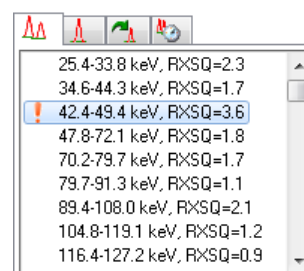
The fit detail panel contains multiple tabs, which may be used to display or edit details of regions, peaks, fitted parameters or the fit history.

Region list tab

The region list tab contains all the fitted regions of the loaded measurement.

The list contains the boundaries of the regions, as well as their Reduced Chi-Squared value.

If this value is greater than 3, a red exclamation mark is placed beside the region, thereby designating problematic areas in the measurement. If you click on a region in this list, the selected region will be displayed in the spectrum window, and a manual refinement may be performed.

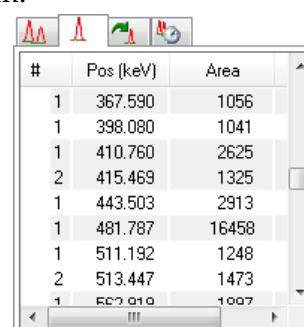


25.4-33.8 keV, RXSQ=2.3
34.6-44.3 keV, RXSQ=1.7
42.4-49.4 keV, RXSQ=3.6
47.8-72.1 keV, RXSQ=1.8
70.2-79.7 keV, RXSQ=1.7
79.7-91.3 keV, RXSQ=1.1
89.4-108.0 keV, RXSQ=2.1
104.8-119.1 keV, RXSQ=1.2
116.4-127.2 keV, RXSQ=0.9

Peak list tab

The region list tab contains the fitted peaks which found in the spectrum.

The row contains basic information about fitted peaks (position or energy, area and its relative uncertainty). As the peaks belong to different consecutive regions, it is advantageous to group them by their regions by utilizing alternating background coloring of the rows. Active region's peaks are displayed with another different background color. If you click on a peak on this list, the selected peak's region will be displayed in the spectrum window, and a manual refinement may be performed.



#	Pos (keV)	Area
1	367.590	1056
1	398.080	1041
1	410.760	2625
2	415.469	1325
1	443.503	2913
1	481.787	16458
1	511.192	1248
2	513.447	1473
1	567.010	1007

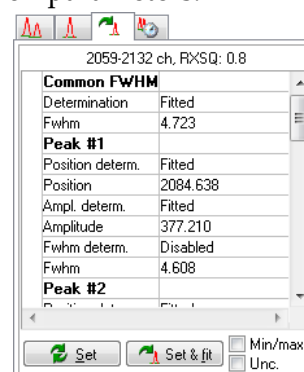
Fit refiner tab

For advanced users, sometimes the versatile refinement tools – provided on the fine tuning toolbar – are not enough, and unconditional access is needed to the region parameters.

The fit refiner tab may serve this purpose, as it allows enabling and disabling, as well as direct editing of fitted parameters.

When you modified a parameter value, and move the cursor to another field, the new model will be immediately drawn in the spectrum window with different colors.

If you want to reset the parameters to their initial value, just click on the original region in the spectrum window: all parameters will be restored.



2059-2132 ch, RXSQ: 0.8

Common FWHM	
Determination	Fitted
Fwhm	4.723
Peak #1	
Position determ.	Fitted
Position	2084.638
Ampl. determ.	Fitted
Amplitude	377.210
Fwhm determ.	Disabled
Fwhm	4.608
Peak #2	
Position determ.	Fitted
Position	2084.638
Ampl. determ.	Fitted
Amplitude	377.210
Fwhm determ.	Disabled
Fwhm	4.608

Set Set & fit Min/max Unc.

The *Set* button will keep the edited values, so these manually edited parameters will be stored and used during reporting. The *Set & fit* button uses the hand-modified parameters only as an initial estimation, and performs a fit from that initial model.

The *Min/max* check box toggles the visibility of parameters' minimum and maximum boundary values. This may be very useful in case of misfits to decide if the problem is because parameters

are at their boundary (e.g. when a faulty FWHM calibration may not even result a proper peak width). The *Unc.* (uncertainty) check box displays the read-only uncertainty fields for each parameter, therefore makes it possible to quickly check whether a parameter is meaningful or not.

Fit history tab

The fit history tab is for advanced users only: it contains all estimated and fitted models for all regions. This is mainly for error tracking purposes, as it may provide information on how the fitting algorithm successively approximated the optimum solution.

8.4.4. Elements of the peak list panel

The peak list panel contains most important details about the suspected and fitted peaks.

Spectrum	Peak details		Messages	Nuclide Id				
Pos (ch)	Pos unc. (ch)	E (keV)	E unc. (keV)	Area (cnt)	Area unc. (cnt)	Area unc. %	FWHM (ch)	
111.954	0.811	30.2292	0.7006	549	274	50.0%	3.9	
147.979	0.284	39.9837	0.6554	13789	402	2.9%	3.4	
154.202	0.571	41.6639	0.6665	890	231	26.0%	3.4	
167.699	0.055	45.3083	0.6431	8700	409	4.7%	3.5	
172.018	0.157	46.4746	0.6426	3215	286	8.9%	3.5	
184.037	0.136	49.7199	0.6375	4093	328	8.0%	2.7	
187.703	0.110	50.7099	0.6357	9864	560	5.7%	2.7	
194.259	0.190	52.4802	0.6344	2436	247	10.1%	2.7	
200.149	0.157	54.0704	0.6314	3372	328	9.7%	2.7	

The list contains Gaussian centroid position, its absolute uncertainty, its energy value together with uncertainty, peak area with absolute and relative uncertainty, fitted FWHM value and its uncertainty.

If efficiency calibration could be loaded automatically, then additional columns detail the efficiency value at the energy of the peak centroid, and relative uncertainty of the efficiency, as well as the efficiency corrected peak area together with its uncertainty (combined from the uncertainty of the peak area and the uncertainty of the efficiency curve at the centroid).

By clicking the *Show selected peak* button, the spectrum window appears, locating the spectrum region of the selected peak.

8.4.5. Elements of the fit fine tuning toolbar

There are several tools on the Fine tuning toolbar to modify a region's automatic deconvolution.



Re-fits the clicked region. Rarely used, only if you suspect that a sub-optimal (unstable) fit is found, where the optimum solution changes when you repeatedly fit the region.



Re-fits the clicked region with automatic peak insertion. Used when a sub-optimal fit is found with a missing peak, but the position of the missing peak is uncertain, and you want to delegate the job of peak position determination to the fitting algorithm.



Inserts a peak into the region, at the clicked position. Used when a sub-optimal fit is found with a missing peak, and the position of the missing peak is suspected by the user.



Deletes a peak from the region, which is located at the clicked position.



Deletes the clicked region with all of its peaks.



Splits a region at the clicked position into two half regions.

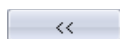


Merges two or more regions. To use this tool, click over the first region and drag the mouse cursor to the last region to be merged (do not release the mouse button).

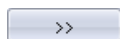
If you have pressed a toolbutton, but it turns out that the fine-tuning is not necessary, just press Esc key to leave the selected working mode.

8.4.6. Elements of the navigating toolbar

Several methods may be used to quickly select a specific region in the Spectrum evaluator. The fastest region and spectrum navigation may be achieved by the Navigation toolbar, which is located at the bottom of the spectrum peak evaluator.



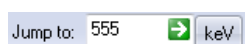
Previous region button: jumps to previous fitted region. Alternatively, you can hit the - key on your keyboard.



Next region button: jumps to next fitted region. To revise fitted regions one after the other, click this button repeatedly. Alternatively, you can hit the + key on your keyboard.



Scroll bar: scrolls to any spectrum region.



Position edit box, Jump button, X axis unit changer: quick location of a specific spectrum portion is achievable by using these positioning tools. Click the unit changer (labeled with “keV” or “ch”) in order to toggle the unit of positioning between channel and energy, then enter the new position, and hit Enter key or click the green jump button to display the spectrum part around the entered position.

If you hit the *Home* key, the beginning of the spectrum will be displayed, while pressing the *End* key shows the last valuable channels.

8.5. Performing spectrum deconvolution

HyperLab's spectrum deconvolution processes the measured single pulse-height gamma spectrum, or two spectrum halves in case of Dual LFC corrected measurement, and produces a peak list for further evaluation. See further details in section “Model functions of peak fitting”.

8.5.1. Performing automatic peak fit

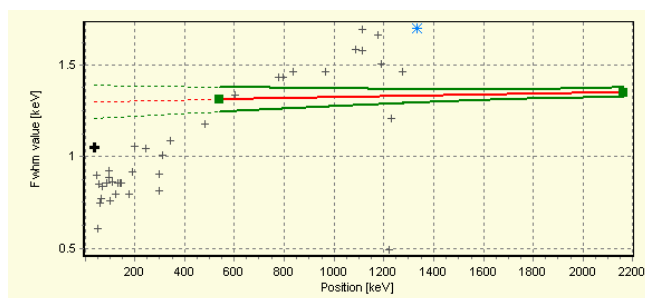
The first step of the deconvolution is to locate the non-background regions of the spectrum, where peaks may occur. This is done by a peak search algorithm, which requires at least a rough *FWHM calibration* (Full Width at Half Maximum) for its convolution function to work.

At least an approximate *energy calibration* is also necessary, because HyperLab switches to Variable peak width method in the vicinity of the 511keV annihilation peak – and naturally for calculating exact peak positions in energy units.

Therefore it is always advisable to check the validity of the calibrations before the deconvolution process.

Checking the FWHM calibration

To display current FWHM calibration, select the *Calibration / FWHM* calibration menu item. Now the FWHM calibration editor window appears. For a quick calibration check, click *Chart* tab at the top.

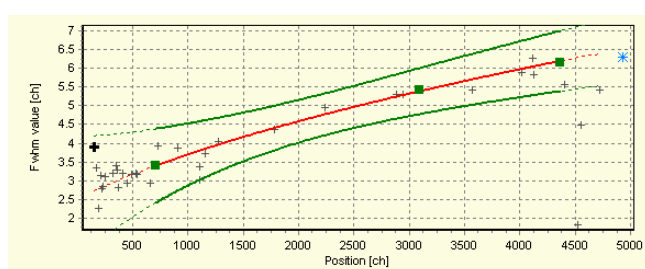


The currently used FWHM calibration curve is displayed here together with filled green squares as FWHM calibration points. HyperLab also estimates the width of the suspected peaks, and displays these values as gray crosses.

The figure shows a case when the FWHM is totally mis-calibrated: it is too high at low energy values, and too low at high

energies. You can easily add proper calibration points by clicking on a gray cross, and then on the *Add* button. The unnecessary point also may be deleted under the tab *Calibration points and function*.

For detailed description of the FWHM editor window, see section “FWHM calibration editor”.



In case of proper FWHM calibration the majority of the suspected peaks' estimated FWHM value is in the neighborhood of the calibration curve.

Please note that large deviations may occur before the deconvolution, even for valid calibration, as peaks' FWHM values are just rough estimations and not fitted values

at this time.

Much better agreement is expected after a successful fit, when FWHM values of the fitted peaks are displayed with gray triangles.

Checking Energy calibration

Exact energy calibration is important for sophisticated tasks, like isotope identification.

However, when only a quick peak list is required for well-known isotopes, a rough energy calibration is enough before fit.

Your energy calibration is proper for fitting if the annihilation peak is in the 509 – 513 keV range. Otherwise select *Calibration / Energy calibration* menu item, and edit the calibration points' position or energy values in order to correct them.

See further details in section “Energy calibration editor”.

Please note that a finer energy calibration may only be constructed when the fit is completed, because exact, fitted peak centroid positions will be then only available.

Starting the automatic peak fit



Click the Autofit button or select *Fit / Start automatic fitting* menu item to initiate a fit for the whole spectrum. A progress window is displayed during the fit, listing the problematic regions, where the Reduced Chi-squared of the fit exceeds the value of 3.0.

After the automatic fit is completed, the counts of the first fitted spectrum region is displayed, along with the fitted curves. The list of the regions is also refreshed on the right, with red exclamation marks beside the problematic regions.

It is advisable to always revise all of the regions at least once, because sometimes unphysical fits provide you a region fit with satisfactory Chi-squared, but the fit may be improved further by a trained spectroscopist. To revise the regions, use the double-arrow button on the navigation toolbar repeatedly, in order to walk through all of the fitted regions.

8.5.2. Manual fit refinements

Although HyperLab has an outstanding quality automatic deconvolution algorithm, it sometimes results in sub-optimal region fits.

This may be due to several reasons:

- it may signal a problem with the quality of the measurement system (noisy amplifiers, improper pole-zero settings etc);
- miscalibration of the FWHM values;
- lack of a well-defined background (this may be the case when extremely complicated multiplets fitted, and no relevant background information is available);
- and naturally minor imperfections in HyperLab's complex fitting algorithm.

The following sections deal with the most frequently occurring bugs and their suggested correction methods.

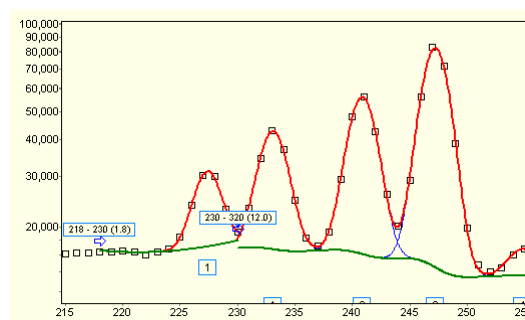
8.5.3. Refinement: merging of improperly split regions

Sometimes HyperLab fails at the difficult task of region bound determination.

This may result in improperly split regions, especially when a multitude of peaks are involved in the fit, which are packed together very closely. In this case the fitter algorithm tries to choose a proper cutting point, and it determines it between two close peaks.

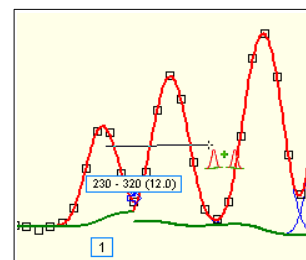
The best tool to eliminate this faulty behavior is the region merge tool.

The figure shows two such regions at channel 230.



To perform the region merge:

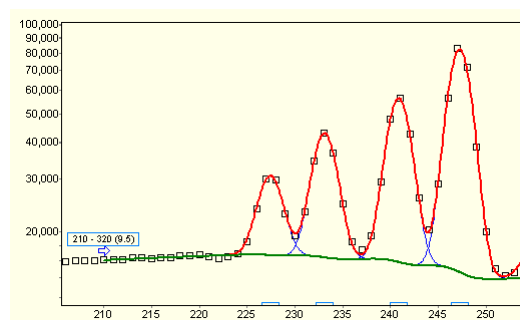
1. Click on the *Region merge* tool on the fit refinement toolbar;
2. click over the first region, and keep the left mouse button pressed;
3. drag the mouse cursor over the second region;
4. release the mouse button.



HyperLab joins the two split regions now, refits them and displays the result.

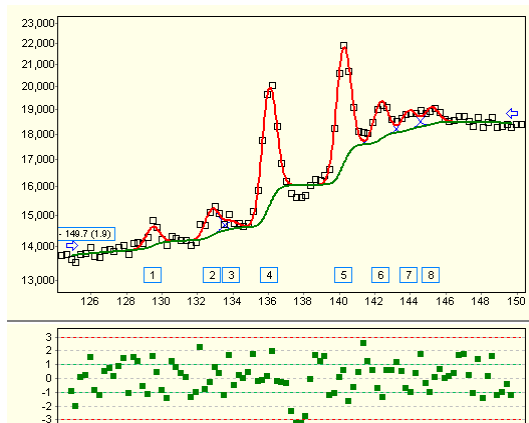
As you can see, the low-energy side of the region also has been moved, in order to find a more stable region background.

The reduced Chi-squared indicates another serious problem, so the peaks rightwards requires a closer inspection.



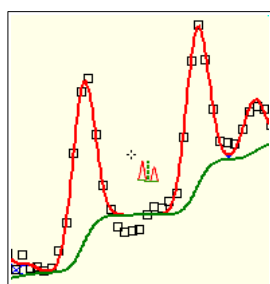
8.5.4. Refinement: splitting of improperly merged regions

Sometimes HyperLab tries to join peaks into one common region, when the background characteristics are not the same under the peaks.



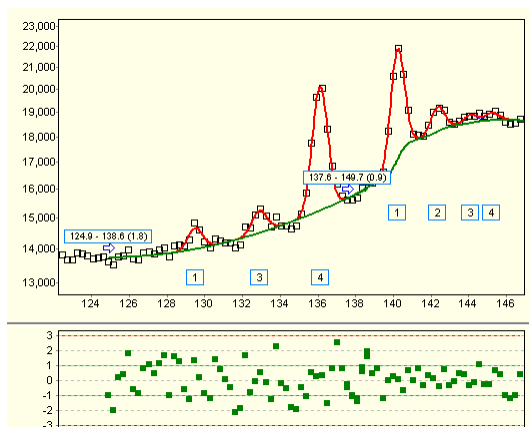
In this case it is advisable to split the region into two or more distinct regions.

The figure shows a region, where a split is suggested at channel 138, because the type of the background drastically changes at this point. The best tool to eliminate this faulty behavior is the region splitter tool.



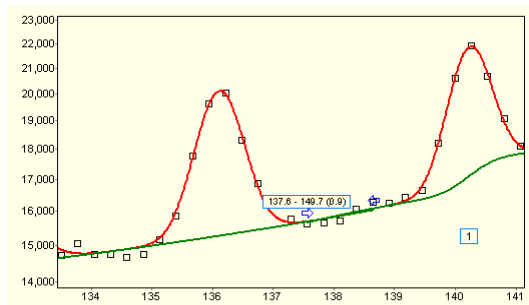
To perform the region splitting:

1. Click on the *Region merge* tool on the fit refinement toolbar;
2. click over the first region, and keep the left mouse button pressed;
3. drag the mouse cursor over the second region;
4. release the mouse button.



HyperLab splits the region now into two halves, refits them and displays the result.

The figure shows the new region bounds around channel 138. Please note that a curved background chosen in the first region, while a stepped one in the second region, therefore the overall Chi-squared became better, and the residual changed to a smoother one.



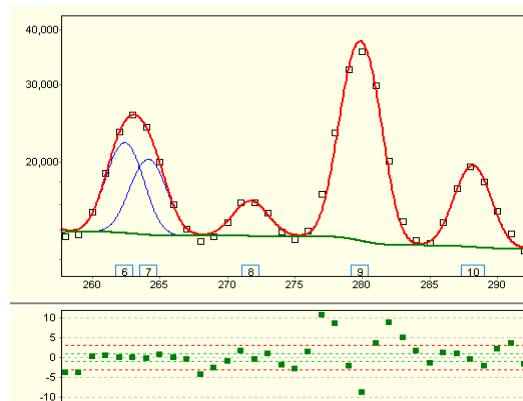
Please take a closer look at the splitting position (use the *Zoom in* tool at the main toolbar). You can see that HyperLab has automatically created *overlapping* region bounds, thus the fit stability has been greatly increased.

8.5.5. Refinement: Missing peaks

When automatic deconvolution determines that the quality of a region fit is not satisfactory, it tries to insert several new peaks into the region, one after the other. This automatic peak where insertion process is stopped when the quality of the fit may not be further improved.

The basis of the peak insertion is the residual, the fitting algorithm seeks for typical shapes of peaks and double peaks.

Sometimes this automatic peak insertion is not successful because in complex multiplets the insertion of a new peak does not always reduce immediately the fit's Chi-squared value. In these cases a significant difference is shown in the residual window, requiring manual inserting of peaks.



You can choose from two peak inserting tools in this case.

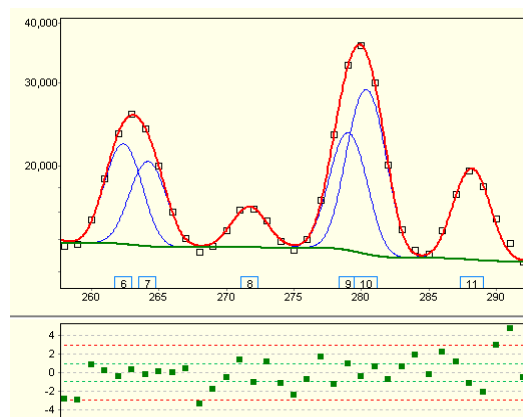


“Refit with auto peak insertion” tool performs a re-fit of the clicked region with a newly added peak, whose position is determined automatically by HyperLab. It is possible that this tool does not result in inserting a new peak, if the fit became worse than before. In this case only manually forced peak insertion may help.



“Manual peak insertion” tool requires you to click at a specific channel where the new peak should be inserted. HyperLab always tries to keep your new peak, even if the fit became worse than before. There is one case, however, when even manual peak addition is canceled: if the peak proves to be non-significant after the re-fit, that is, its amplitude is too small in absolute value; too small compared to the background or to the amplitude uncertainty; or the peak slips too close to another peak.

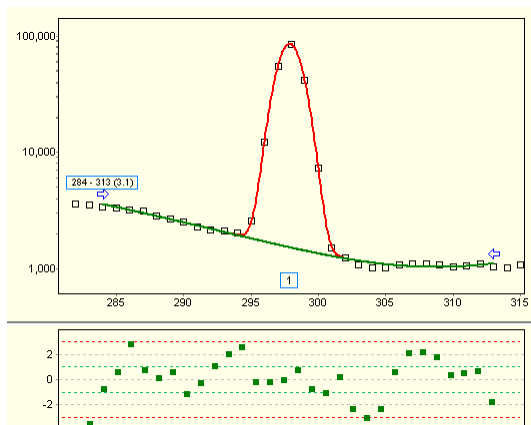
After clicking at channel 277 with the manual peak insertion tool, a new peak is inserted there and a re-fit is performed. The manually specified peak position is not hold fixed, but fitted by HyperLab's nonlinear minimizer in the usual way. Please note that the residual has become significantly smoother, and the peaks have disappeared from it – but a closer look may reveal that possibly another peak may be added at channel 291.



Several peaks also may be inserted in one-step: hold down the Ctrl key, when you click over the channel where the first peak must be added; repeat this Ctrl-click wherever the insertion of peaks may be required, then finish the multiple selection over the last peak *without* the Ctrl key. After the last click, all the selected peaks will be added to the model, and it is re-fitted.

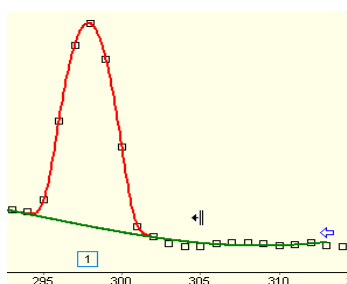
8.5.6. Refinement: adjusting improper region bounds

There may be several cases, when HyperLab's default region bound determination is considered sub-optimal by the spectroscopist.



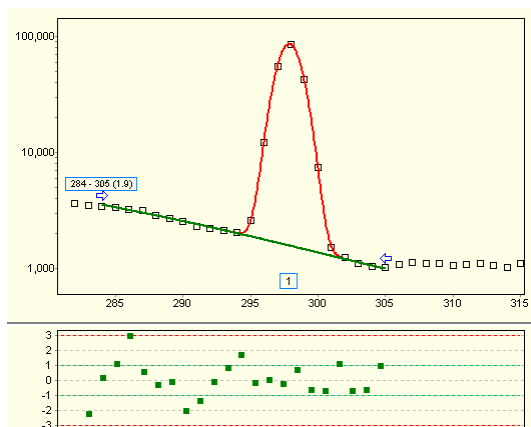
The figure depicts a well-fitted peak, but HyperLab did not notice the change in background type after channel 305. The residual and the high Chi-squared value (3.1) designates the possible problem with the fit.

If you take a closer look at the background, you can observe the sharp changing at the right side. The modification of the background boundary is suggested in this case, so let us try to move the right region boundary leftwards.



Click on the blue arrow at the right boundary of the fitted region, and drag it to its new position, e.g. to channel 305.

When you release the mouse button, HyperLab modifies the fit model, performs a refit and displays the new region.



The region's right bound has changed, and also a different background function is used. The improved Chi-squared value shows the better fit. If you look at the left side of the region, you will notice that the same problem of changing background may occur there, so it is worth a try moving the left region limit to channel 288.

After that change, the Chi-squared may be even lower, and non-random tendencies will mostly disappear from the residual.

If you are not satisfied with the results, just click the *Undo* button, and your previous fit will be restored.

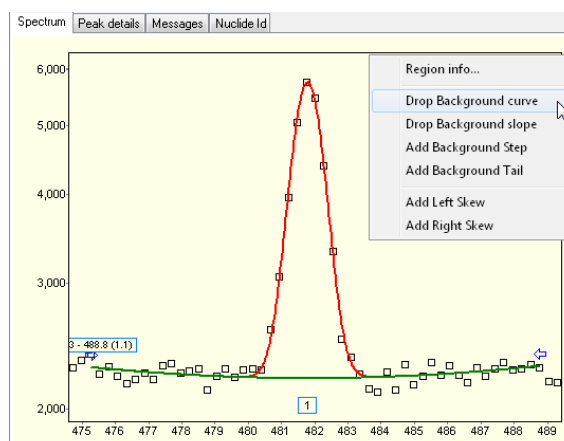
8.5.7. Refinement: dropping unnecessary peak parameters

After HyperLab found an optimum model for the fitting problem, it eliminates unnecessary (insignificant) fitting parameters. Basis of the elimination may be too small value, too small value compared to its uncertainty etc.

Sometimes this logic does not drop parameters which are unnecessary for a good fit, and user intervention will be required – or simply two models fit well to a specific region, and the spectroscopist would choose a model which was not preferred by the automatic fitter.

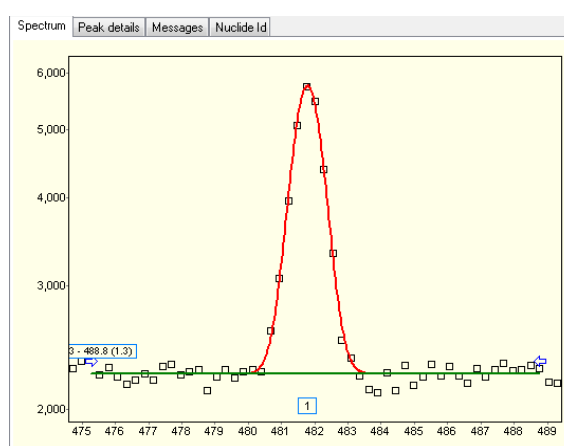
The figure shows a region where the algorithm chooses a significant step for the background, but one can suspect that another model without a step would also fit well to the measured counts.

To eliminate the step parameter from the region's fitted model, right-click the region. A popup menu appears now, providing the parameters that may be eliminated. Choose *Drop Background Step* menu item.



HyperLab now eliminates the step, refits the region and displays the new fit.

The Chi-squared value increased (from 1.1 to 1.3), showing why the automatic fitter inserted the step previously.

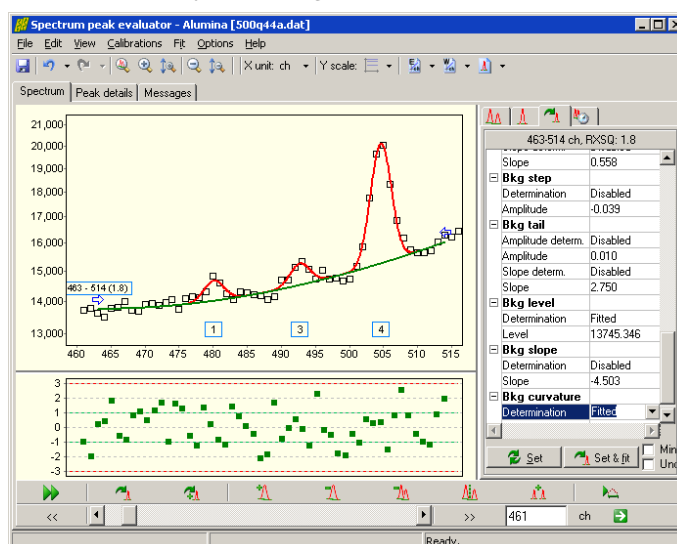


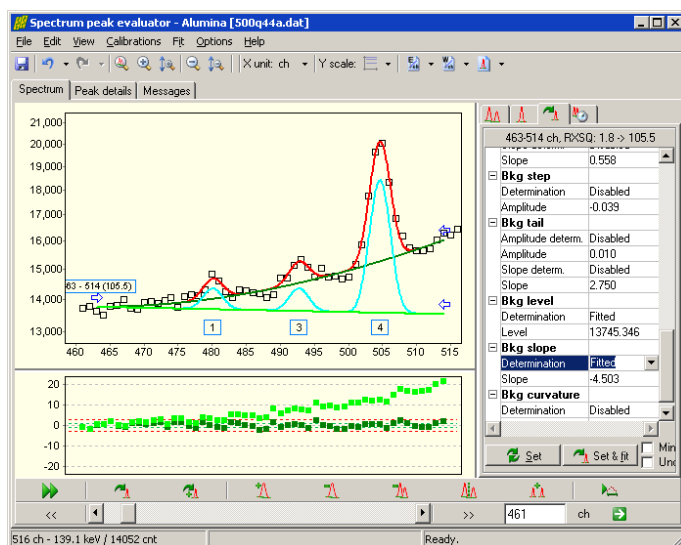
8.5.8. Refinement: manual modifying of the fit model

This example shows manual modifying of the fit model by utilizing the fit refiner tab.

This alumina spectrum has a region where HyperLab fitted a background curve (2nd order member of the background polynomial), and completely eliminated the slope (1st order member). If you are curious if the fitted curve is necessary, or it may be replaced by a slope, follow the steps below:

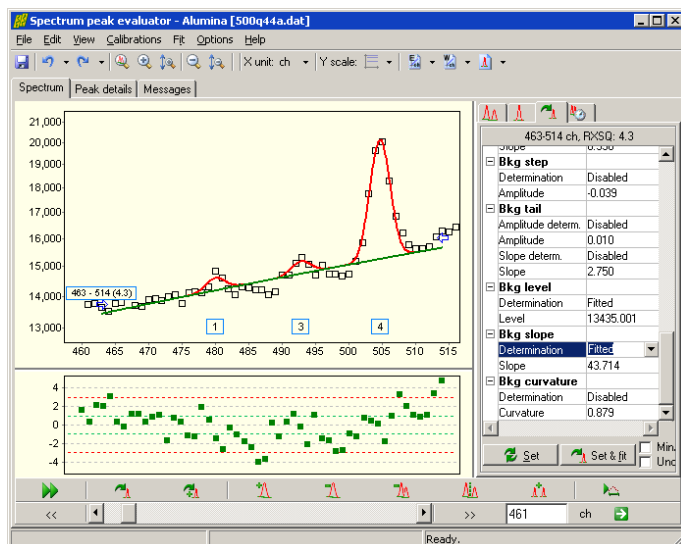
- switch to the fit refiner tab,
- change *Bkg curvature* to “disabled”;
- change *Bkg slope* to “enabled”;
- click *Set & fit* button.





When you manually modify a parameter of the fitted region (and change to another editor field), HyperLab automatically displays the new model with a different color scheme. This way you can immediately check the new model. This is, however, only a visual representation, and the entered data is not used elsewhere until you click one of the **Set** or **Set & fit** buttons.

As a new fit is required now, the **Set & fit** button should be clicked, therefore the manually set values are used only as an initial estimate for the fit.



After the fit, the new model is displayed with a background slope instead of a curve. Chi-squared changed from 1.8 to 4.3, so in this case the experiment showed that the slope is a worse parameter to fit the background than the curve.

Click **Undo** button to restore the previous fit now.

8.6. Peak evaluation algorithm settings window

This form contains all settings required to tailor the peak evaluation algorithm to your needs. It is available either from the database record editor of the peak evaluation algorithm setting records, or from the peak evaluation module. Use the tabs at the top of the form to switch to a specific settings category. About peak fitting functions, see “Model functions of peak fitting”.

8.6.1. Generic tab

The generic tab contains most commonly changed generic evaluation algorithm settings.

Peak search thresholds

For spectrum peaks

Peak search sensitivity within the spectrum. Default value is 3.0.

For residual peaks

Peak search sensitivity within the residual. Default value is 3.0.

Region bound determination

Max No. of initial peaks

Contains the upper limit for the number of peaks used to set up an initial region for the fit. Default value is 10.

Region extending for peaks

Region bound limits where peaks merged into an initial region. Expressed as a multiplier for current FWHM. Default is 10.

Region bound extending for kg

Left and right wing for region, used for background determination. Expressed as a multiplier for current FWHM. Default value is 1.25.

Automatic peak insertion

Enable automatic peak insertion during refit

Determines if peak evaluator will try to improve the fit automatically by inserting new peaks to the region's most probable locations and run a refit. Default value is Enabled.

Max peak insertion trials

Maximum number of peak insertion trials. Default value is 10.

Minimum peak amplitude

No fitted peak amplitude is allowed to be less than this value (in counts). Default value is 5.0 counts.

Peak insertion RXSQ limit

Lowest reduced Chi-squared value for the fit when refit takes place. Default value is 0.5.

Automatic curve, tail, step disabling

Disable curve, tail and step for 'small peak-only' regions

Disables unnecessary peak parameters in case of regions where only small peaks may be found. Default value is Enabled (that is, disabling is in effect).

Small peak amplitude limit

Maximum peak amplitude where a peak is considered to be 'small'. Default value is 500 counts.

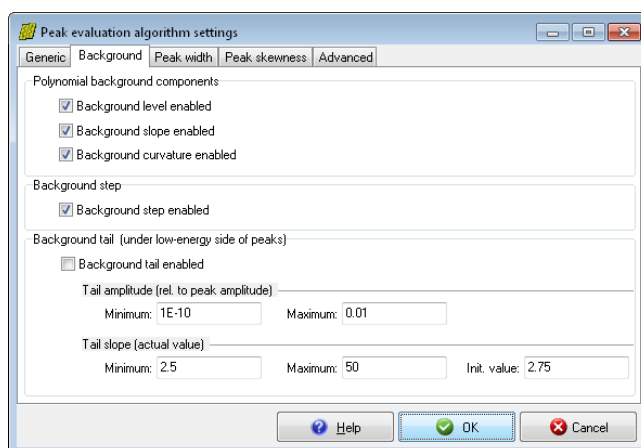
Evaluation cut-off

Start evaluation from

Minimum peak evaluation energy value in keV, where the automatic evaluation starts. Helps to get rid of disturbed low-energy regions for routine evaluations.

8.6.2. Background tab

The background tab contains settings for background components under regions.



It affects the the polynomial background, the step under peak centroid as well as the long background tail on the low-energy side of the peaks.

Polynomial background components

Background level enabled

Zeroth order component of polynomial background function. Almost always fitted. Default value is Enabled.

Background slope enabled

First order component of polynomial background function. Default value is Enabled.

Background curvature enabled

Second order component of polynomial background function. Default value is Enabled.

Background step

Background step enabled

Step function which jumps under the peak centroid. Default value is Enabled.

Background tail

Background tail enabled

If enabled, peak evaluator tries to fit a long, skewed background function under the low energy side of the peak, which also contributes to the fit also far away from the peak centroid. As this phenomenon is observable mainly for older detectors only, it is disabled by default. The bigger is the tail, the less is the area of the peaks in the region. Default value is Disabled.

Tail amplitude minimum

Lower limit of tail amplitude, relative to peak amplitude. Default value is 1e-10; should not be less than this value.

Tail amplitude maximum

Upper limit of tail amplitude, relative to peak amplitude. Default value is 0.015; should not be higher than this value.

Tail slope minimum

Lower limit of tail slope. Default value is 2.5; should not be less than this value.

Tail slope maximum

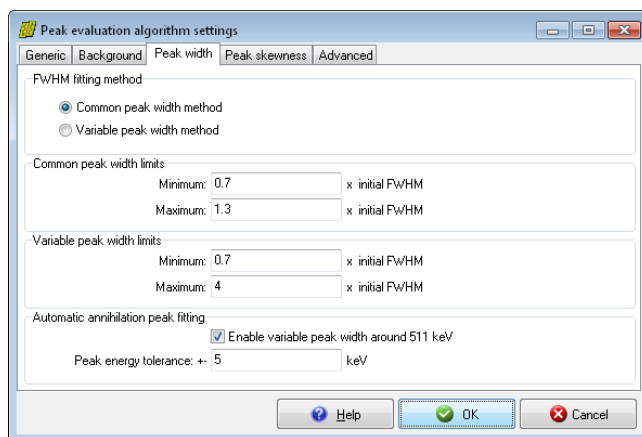
Upper limit of tail slope. Default value is 50.

Tail slope initial value

Value of tail slope used initially when starting a region fit. Must be between Minimum and Maximum values. Default value is 2.75.

8.6.3. Peak width tab

The peak width tab contains settings regarding the fitted FWHM of the peaks.



FWHM fitting method

Common peak width method

Fits one common FWHM value for each peak within a region. This is a proper setting for most regions, where FWHM does not change significantly. The common FWHM setting significantly speeds up fitting, and results in very stable fits.

Variable peak width method

Fits FWHM individually for each peak within a region. This is rarely selected, when users experience problems due to broadening peaks. Variable FWHM setting significantly slows down fitting, and may result in erroneous fits, because peak width may vary from extremely narrow to extremely wide. However, this is required when one region contains peaks with very different FWHM values, e.g. annihilation peaks with regular ones. The Common peak width method is the default.

Common peak width limits

Minimum

Low limit for FWHM for 'Common peak width method'. Relative value to that of calculated from current FWHM calibration.

Default value is 0.7 (FWHM is allowed to varyate -30% below the current FWHM value).

Maximum

High limit for FWHM for 'Common peak width method'. Relative value to that of calculated from current FWHM calibration.

Default value is 1.3 (FWHM is allowed to varyate +30% above the current FWHM value).

Variable peak width limits

Minimum

Low limit for FWHM for 'Variable peak width method'. Relative value to that of calculated from current FWHM calibration. Default value is 0.7 (FWHM is allowed to varyate -30% below the current FWHM value).

Maximum

High limit for FWHM for 'Variable peak width method'. Relative value to that of calculated from current FWHM calibration. Default value is 4.0 (FWHM is allowed to reach 4 times the current FWHM value - for extremely broadened peaks).

Automatic annihilation peak fitting

Enable variable peak width around 511 keV

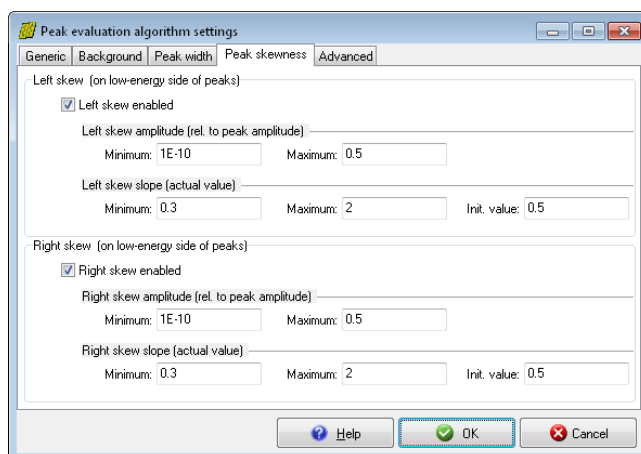
Automatically switches to 'Variable peak width method' around the 511.0 keV annihilation peak. Default value is Enabled.

Peak energy tolerance

Specifies the energy tolerance relative to 511.0 keV, where automatic switch should take place. Default value is ± 5.0 keV.

8.6.4. Peak skewness tab

The peak skewness tab contains settings for fits that control skewness of the peaks.



It contains two panels: one for skew on the low-energy side of the peak (left skew), and one for the high-energy side of the peak (right skew).

Left skew (on low-energy side of peaks)

Left skew enabled

If enabled, the peak evaluator tries to incorporate a relatively sharp peak function into the low energy side of the peaks, which decreases rapidly close to the peak centroid. This peak function is able to describe the slight broadening of the Gaussians' left bottom. The area of the left skew is also added to the reported peak area. Default value is Enabled.

Left skew amplitude minimum

Lower limit of Left skew amplitude, relative to peak amplitude. Default value is 1e-10; should not be less than this value.

Left skew amplitude maximum

Upper limit of Left skew amplitude, relative to peak amplitude. Default value is 0.75 .

Left skew slope minimum

Lower limit of Left skew slope. Default value is 0.3 .

Left skew slope maximum

Upper limit of Left skew slope. Default value is 2.0; should not be less than this value.

Left skew slope initial value

Value of Left skew slope used initially when starting a region fit. Must be between Minimum and Maximum values. Default value is 0.5 .

Right skew (on high-energy side of peaks)

Right skew enabled

If enabled, the peak evaluator tries to incorporate a relatively sharp peak function into the high energy side of the peaks, which decreases rapidly close to the peak centroid. This peak function is able to describe the slight broadening of the Gaussians' right bottom. The area of the Right skew is also added to the reported peak area. Default value is Enabled.

Right skew amplitude minimum

Lower limit of Right skew amplitude, relative to peak amplitude. Default value is 1e-10; should not be less than this value.

Right skew amplitude maximum

Upper limit of Right skew amplitude, relative to peak amplitude. Default value is 0.75

Right skew slope minimum

Lower limit of Right skew slope. Default value is 0.3.

Right skew slope maximum

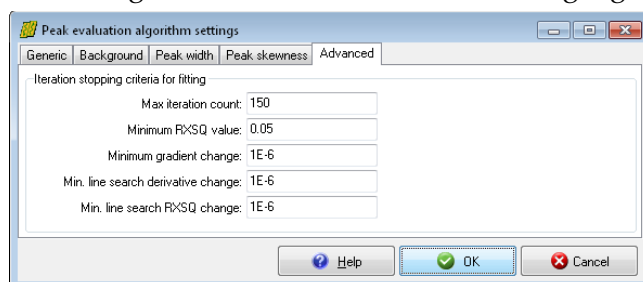
Upper limit of Right skew slope. Default value is 2.0; should not be less than this value.

Right skew slope initial value

Value of Right skew slope used initially when starting a region fit. Must be between Minimum and Maximum values. Default value is 0.5.

8.6.5. Advanced tab

The advanced tab contains settings to fine tune the nonlinear fitting algorithm.



Change the defaults with caution, as improper values may lead to sub-optimal deconvolution process.

Iteration stopping criteria for fitting

Max iteration count

Upper limit for number of iterations for nonlinear fitter. Default value is 300. Less than this value may cause non-optimal fit results.

Minimum RXSQ value

Lower limit for reduced Chi-squared, when nonlinear fitter should quit unconditionally. Default value is 0.05 (this is almost never reached).

Minimum gradient change

Lower limit for gradient value change. If the gradient of fitted parameters changes to less than this value between iterations, then iteration will be stopped. Default value is 1e-9 (should not be greater than 1e-6).

Minimum line search derivative change

Lower limit for derivative value change. If the derivative of fitted parameters changes to less than this value between line search iterations, then iteration will be stopped. Default value is 1e-5.

Minimum line search RXSQ change

Lower limit for reduced Chi-squared value change. If the reduced Chi-squared changes to less than this value between line search iterations, then iteration will be stopped. Default value is 1e-6.

8.7. Peak area and area uncertainty calculation

From HyperLab version 2005, a fine-tuned peak area uncertainty calculation method is applied, which is described in this section.

Objective function for fitting

During the spectrum fitting, we try to fit a sum of peak, skew and background functions to the measured counts. The standard Chi-Squared used as a merit function for the goodness of fit:

$$F = \sum_{j=1}^n \frac{(Count_j - Y_j)^2}{\text{var}(Count_j)}$$

where

$Count_j$	Measured count in the j'th channel of the region
$\text{var}(Count_j)$	Variance of the measured count at j
Y_j	Sum of peak and background functions at j
n	Number of channels in the region

Calculation of the peak area

If the fit reaches a minimum, peak area is calculated from the actual values of the fitted and/or fixed parameters:

$$Area = GAmpl \cdot GWidth \cdot \sqrt{\pi} \cdot (1 + LSAmpl \cdot LSSlope \cdot GWidth + RSAmpl \cdot RSSlope \cdot GWidth)$$

where

$GAmpl$	Gaussian Amplitude
$GWidth$	Gaussian width (FWHM / 1.6651)
$LSAmpl$	Left Skew Amplitude
$LSSlope$	Left Skew Slope
$RSAmpl$	Right Skew Amplitude
$RSSlope$	Right Skew Slope

8.7.1. Uncertainty of fitted parameters

After the fit, also M , the inverse of the covariance matrix of the fitted parameters is computed:

$$M_{kl} = \sum_{j=1}^n \left(\frac{1}{\text{var}(\text{Count}_j)} \cdot \frac{\partial F}{\partial p_k} \cdot \frac{\partial F}{\partial p_l} \right)$$

Inverse of M (the covariance matrix) contains the covariances of the fitted parameters:

$$\text{cov}(p_k, p_l) = (M^{-1})_{kl} \quad k \neq l$$

And their variances

$$\text{var}(p_k) = (M^{-1})_{kk}$$

where

$\frac{\partial F}{\partial p_k}$	partial derivative of Chi-squared by fitted parameter p_k
M^{-1}	covariance matrix (inverse of M)
$\text{cov}(p_k, p_l)$	covariance between parameters p_k and p_l
$\text{var}(p_k)$	variance of parameter p_k

8.7.2. Uncertainty of Peak Area

Variance of the area is computed by a standard error propagation method. This method is well known, and provides the overall uncertainty of arithmetic expressions, which in turn depend on other uncertain values themselves.

The calculation incorporates

- the uncertainty of the fitted parameters, and
- the dependence of the peak area on the individual uncertain parameters

$$\text{var}(\text{Area}) = \sum_{k,l} \frac{\partial \text{Area}}{\partial p_k} \cdot \text{cov}(p_k, p_l) \cdot \frac{\partial \text{Area}}{\partial p_l}$$

where

$\text{var}(\text{Area})$	variance of peak area
$\frac{\partial \text{Area}}{\partial p_k}$	partial derivative of the peak area by fitted parameter p_k

According to our Monte-Carlo simulations, this approximates the real peak area uncertainties very well.

You are able to check this calculation using

- the covariance matrix of the fitted parameters, which may be displayed in HyperLab for each region by the “File / General info” menu in HyperLab’s Peak evaluator module,
- and calculating the partial derivatives of the Peak Area using the following expressions:

Fitted parameter (p_k)	$\frac{\partial \text{Area}}{\partial p_k}$
GAmpl	$G\text{Sig} \cdot (1 + G\text{Sig} \cdot (L\text{SAmpl} \cdot L\text{SSlope} + R\text{SAmpl} \cdot R\text{SSlope})) \cdot \sqrt{\pi}$
GWidth	$G\text{Ampl} \cdot (1 + 2 \cdot G\text{Sig} \cdot (L\text{SAmpl} \cdot L\text{SSlope} + R\text{SAmpl} \cdot R\text{SSlope})) \cdot \sqrt{\pi}$
LAmpl	$G\text{Ampl} \cdot G\text{Sig}^2 \cdot L\text{SSlope} \cdot \sqrt{\pi}$
LSSlope	$G\text{Ampl} \cdot G\text{Sig}^2 \cdot L\text{SAmpl} \cdot \sqrt{\pi}$

Fitted parameter (p_k)	$\frac{\partial Area}{\partial p_k}$
RSAmpl	$GAmpl \cdot GSig^2 \cdot RSSlope \cdot \sqrt{\pi}$
RSSlope	$GAmpl \cdot GSig^2 \cdot RSAmpl \cdot \sqrt{\pi}$

8.7.3. Comparison with conventional Peak Area calculation method

In most cases, other gamma spectrometry applications calculates the uncertainty of the peak are based on the following model:

$$\sigma_s = \sqrt{G + \left(\frac{N}{2n}\right)^2 (B_1 + B_2)}$$

The model assumes a singlet peak, where a linear background region lies beside the peak, both on the left and the right sides, with

σ_s	uncertainty in peak area
G	gross counts under the peak (background + peak counts)
N	number of channels under the peak
n	number of channels both on the left and right sides
B_1, B_2	background counts on the left and right side

This approach is more or less valid, however if too narrow background region is used, the uncertainty estimations will be unnecessarily high, as this is the case of most evaluation software.

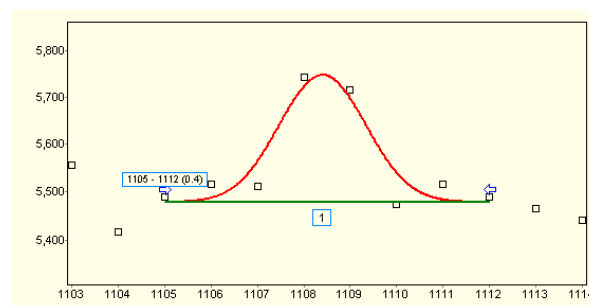
HyperLab is superior to this simple method due to the followings:

- intelligently extends the region as far as possible, thus minimizing the uncertainty
- its uniform calculation expression may be applied to every region, even for multiplets (in spite of different expressions used for singlet and multiplet cases, as can be seen in other applications)
- may take into consideration a complex (curved and/or stepped) background
- takes into consideration of the reliability of the fit (due to the partial derivatives of the fitted parameters at the minimum).

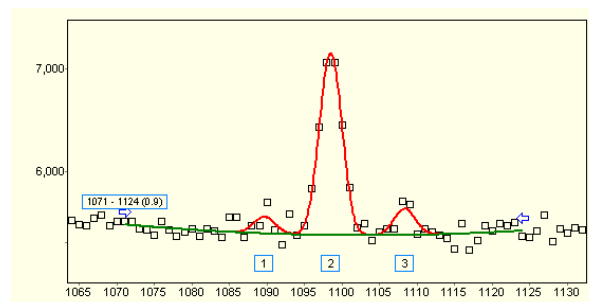
Although HyperLab applies a very different (but otherwise standard) method for peak uncertainty calculations, the calculated values agree very well with other applications, if comparable fitting situations regarded.

Calculation example

A typical fit of a small peak can be seen on the figure below, which contains a singlet-peak fit. The reference uncertainty equation and HyperLab's uncertainty calculation method approximately serves the same 44% area uncertainty value. This shows that the two formulas results in nearly identical results under the same conditions.



HyperLab could reproduce this fit only after manual interventions, as it uses much wider background region during the automatic fit:



In comparison, HyperLab's automatic fit results in 27% area uncertainty for peak No. 3 (the same peak as in the previous example). This lower value can be explained by the followings:

- a much wider the background region utilized,
- thus the nonlinear fitter finds a minimum with greater confidence,
- therefore the uncertainty of the fitted parameters will be smaller,
- so the uncertainty value of the peak area will also be significantly lower.

9. Visual Nuclide Identification

HyperLab has a powerful quantitative isotope identification module, which reliably identifies a large set of nuclei found in its nuclear database, determining activities of isotopes with overlapping peaks, while presenting the results in an exceptionally enjoyable visual manner. This utility is also able to perform the identification on virtually any kind of gamma-spectrum producing phenomenon, e.g. prompt-gamma activation reactions, if the gamma intensity ratios are constant within a component to be identified.

Nuclide identification results

In HyperLab, the result of the nuclide identification is a list of activity concentrations or intensities for each component determined.

Components in HyperLab terminology may mean any kind of material, which provides a gamma line set with fixed relative intensities. The most common component is the radioactive decay. Other example would be any kind of gamma-producing reaction, e.g. the prompt-gamma capture, where the intensity ratios of the individual gamma lines are also constant within a capture reaction.

HyperLab's important concept is to **fit the activity of all components together** for a spectrum, and not activities at the individual components or spectrum peaks. Thus you will not see averaged activities calculated individually for each spectrum peak, just one common activity value, which is fitted to all of the peaks of all component at once.

Beside the activity concentrations, **MDA values** are also computed for gamma lines and for each component.

Requirements for nuclide identification

- **Well-calibrated measurement.** In HyperLab's present version, only one measurement can be used for nuclide identification at a time. That measurement should have a relatively precise energy calibration, thus creating and using a nonlinearity curve is strongly recommended.
- **Efficiency curve.** An absolutely calibrated efficiency curve is a requirement, if you want to get absolute component activity values in kBq (this is the case almost every time). If you have only relative efficiency curves, the nuclide identification can be performed, too, but the resulting values will be only dimensionless intensities.
- **Nuclear data.** In case of decays, it is already in the database upon initializing. For prompt-gamma (or other, reaction-based) identification, you should import the reactions to your database. We are providing a default PGNAAL library in the form of textual representation of reaction data, which can be installed by the user. These serve also an example for user-creatable reaction libraries.

9.1. Performing nuclide identification

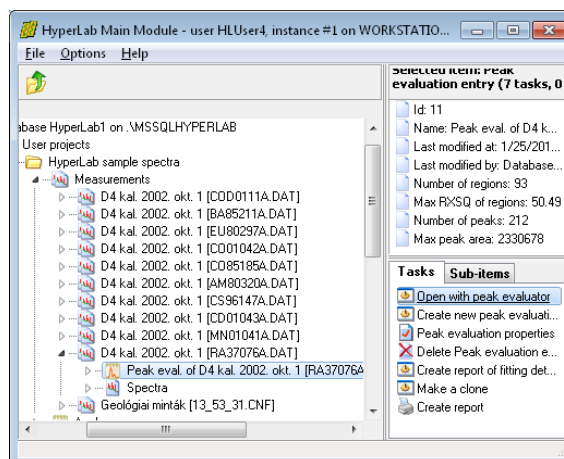
We are demonstrating the capabilities of the nuclide identification module on the sample spectrum of the ^{226}Ra source, named RA37076A.

- Please make sure that you have created a proper nonlinearity curve (for precise energy values) and a proper efficiency curve from the sample measurements.
- Also make sure that you have designated the your efficiency curve as a default for the measurement setup where it was taken. See details in section "Designating a proper efficiency curve as a default".

To start nuclide identification, open the measurement node of RA37076A, select the peak evaluation under it.

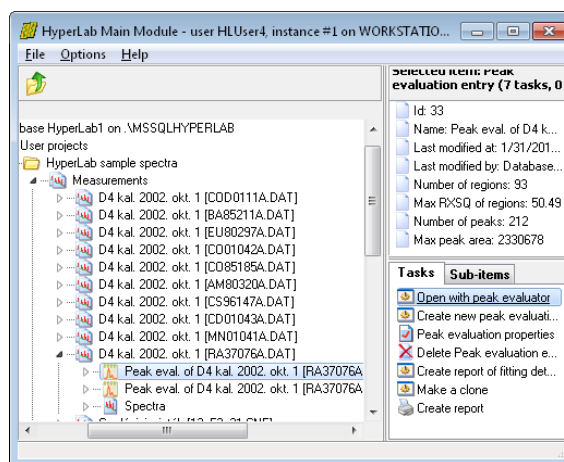
When you double-click on it, the peak evaluator tries to open it. However, it was already used in nonlinearity as well as efficiency analysis, and that made it read-only. This is why a warning message window appears now.

As we possibly want to refine the deconvolution results by the help of the nuclide identification, it is advantageous to skip the loading of that read-only peak evaluation, and create a clone of it, which can be freely modified.



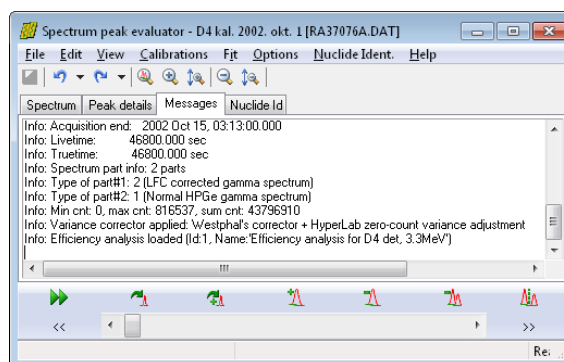
To clone the peak evaluation, select it on the left, and click on the task *Make a clone* on the right pane. After a few seconds, a second peak evaluation appears under the measurement.

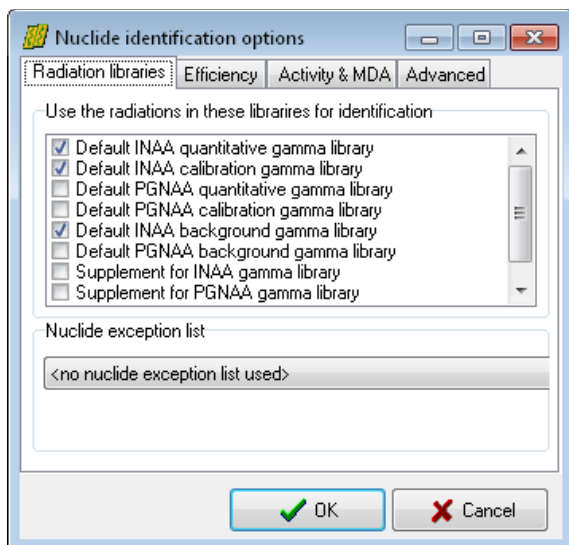
As the peak evaluations ordered from the newest to the oldest by default, select the upper one for processing (if you are in doubt, check the date of the last modification on the upper right pane). Open it with the peak evaluator by a double-click.



After the peak evaluation loaded, please immediately go to the Messages panel, and check that if the efficiency analysis is loaded automatically for the measurement. This is indicated in the last a message line.

If this is not the case, please close the peak evaluator, and follow the steps of the section "Designating a proper efficiency curve as a default" to create such an assignment.

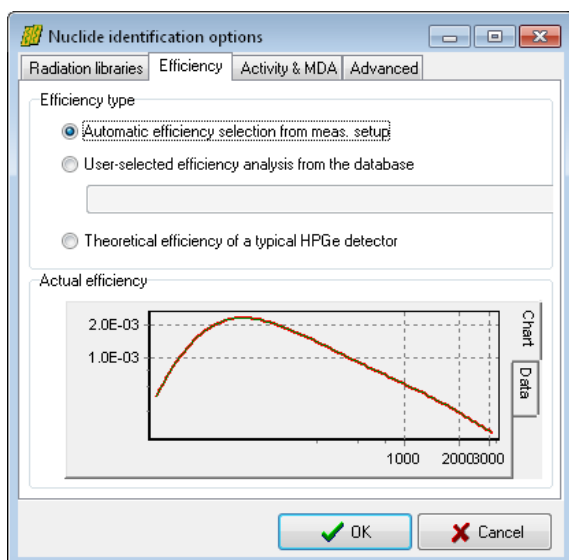




Select *Option / Nuclide identification* menu now, to check current settings.

Under *Radiation libraries* tab, you can select which radiation libraries should be involved in the nuclide search. At the bottom, it is possible to select one from the user defined nuclide exception lists.

For a regular decay measurement, it is not needed to modify these default settings.

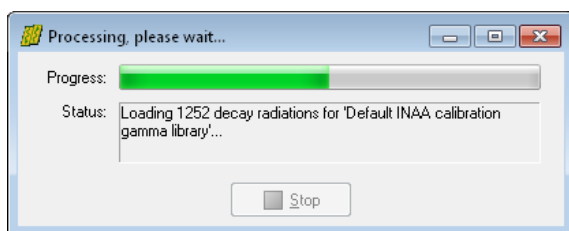


Under the second tab, Efficiency, click on the 'Automatic efficiency selection from meas. setup' item.

If you properly set up your efficiency curve – measurement setup assignment earlier, then the efficiency curve will be immediately displayed at the bottom, which is belonging to the loaded measurement.

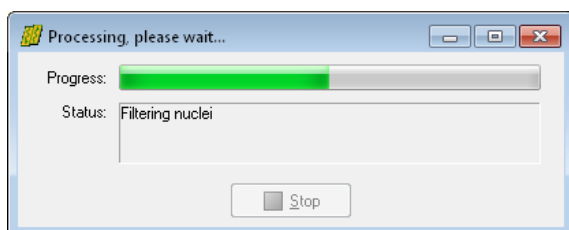
Now click OK.

This efficiency setting will be retained for next sessions, so the nuclide identification will be even more convenient next time.



Now the nuclide identification module loads the nuclear data necessary for the evaluation.

Please wait until the message disappears, then select *Nuclide Ident. / Start identification* menu.

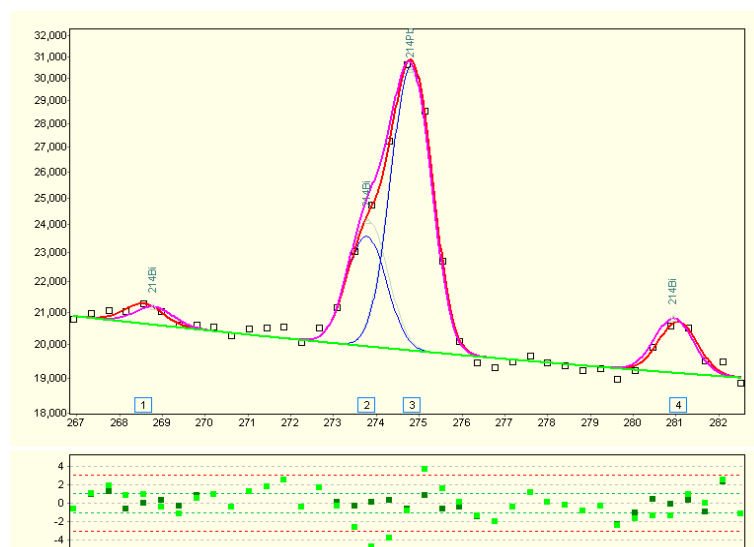


Now the nuclide identification starts, which may last just a few seconds on a reasonable fast computer. After the identification, the computed spectrum of the fitted nuclei will be displayed graphically.

As you walk through the fitted regions of the spectrum, you can see the result of the simulated spectrum.

The following display elements will be used:

- The deconvoluted peak curves are remained in red, the virtual peaks computed from the nuclide identification displayed in magenta color.
- The deconvoluted background is green, while the background from nuclide id is displayed in lime color.
- Individual peaks in a multiplet are blue, but the same peaks from nuclide id is displayed in grayish-green.
- The difference values in the residual window are green rectangles for the spectrum fit, and lime for the nuclide identification fit.



This region contains ^{214}Bi and ^{214}Pb lines, and two lines were in a properly separated multiplet.

In this region, you can immediately observe the followings:

- The energy calibration is well defined. This is imminent as peaks from the nuclide identification always placed at the location of the library energies, while the spectrum peaks are drawn at the fitted channel content, and there is a very good agreement in the peak centroid positions.
- The efficiency calibration seems to be OK, as the intensities (amplitudes) of the nuclide id and the deconvoluted peaks are practically the same.
- HyperLab's nuclide id is easily able to resolve multiplets originating from the same or from different nuclei.

Creating a nuclide identification report

Creating a report with all of the nuclide identification results requires no different action then in case of regular peak reporting: just select File / Create report menu, and the regular peak list report will also contain the results of the nuclide identification

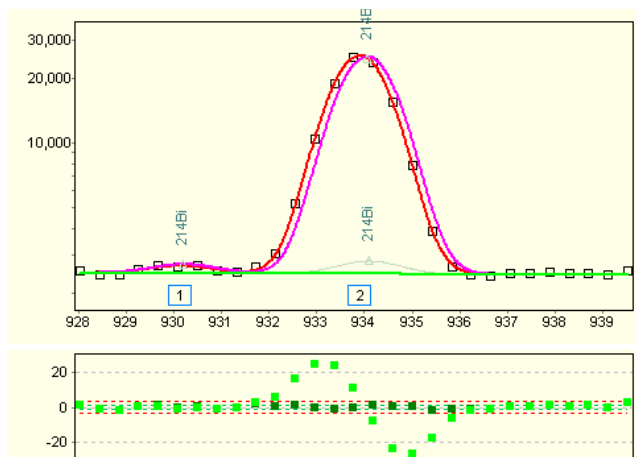
left. Thus the abandoned component will be included in the nuclide list again, and a nuclide identification re-fit occurs.

Energy calibration shift

When a slight difference can be observed in the position of the virtual peaks (displayed by the nuclide identification module) and the measured peaks, probably there is a small energy calibration problem.

Update your calibration, by adding this peak to the energy calibration points, and check if the nonlinearity part of the calibration is in effect.

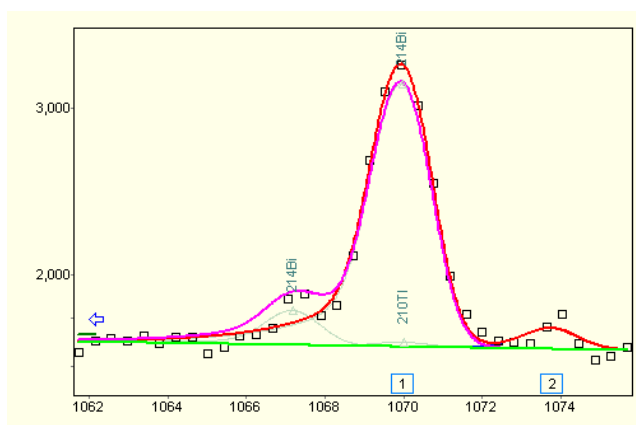
There is a small chance, too, that the nuclear data is not perfect, but this is rarely the case.



Non-fitted spectrum peak found by Nuclide Id

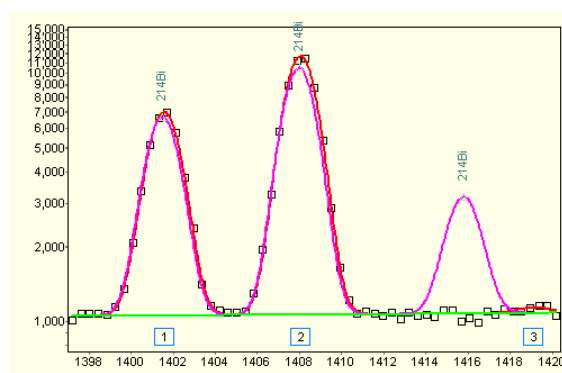
Due to statistical nature of the measured counts, the spectrum peak deconvolution algorithm sometimes misses a peak. In several cases, those peaks are pointed out by the nuclide identification algorithm, as it utilizes the information from all peaks of the nuclide.

The picture shows the case when a small ^{214}Bi peak is missed by spectrum analysis, but the nuclide identification found it. Insert the missing peak manually to the region, and re-run nuclide identification.



Problem with the nuclear data

In some very rare cases, the nuclear libraries are not perfect: may contains errors for the energy positions or the intensities of library peaks. One such example can be seen on this figure. As we see that while intensities and the positions of other ^{214}Bi peaks are properly matching the measured peaks, there is a true outlier at 1416keV. This is probably comes from an intensity problem in the original nuclear data.



9.3. Common problems during nuclide identification

Although nuclide identification is very straightforward with HyperLab, there are a few typical issues which can be easily addressed by the following tips.

Improper energy calibration

If you experience a poor quality nuclide identification, please always check if

- the linear energy calibration is properly done, and
- you are applying a nonlinearity calibration beside the linear one.

Improper efficiency curve selected

In case of the peak intensities of the nuclear library shows large deviations from the fitted peaks, always check that you are using the proper efficiency calibration curve, that is, which is prepared for the same measurement setup, and it is created more or less at the time when your measurement was taken.

9.4. Algorithm of the nuclide identification

The following sections describe the individual steps taken by the nuclide identification algorithm.

Loading of basic data

In this phase we are collecting all the information necessary for the actual nuclide identification. These include

- Peak list, which contains the spectrum peaks to be identified. Every peak has energy, energy uncertainty, area and area uncertainty values.
- List of searched components.
- Radiations belonging to the component. Every radiation must have energy, energy uncertainty, intensity, intensity uncertainty values.
- Detector efficiency curve.

Preliminary search and filtering of peaks and components

The process of matching of peaks and library lines is the following:

- Searching for all radiations, which may belong to a spectrum peak. This is done by searching of radiations, where the uncertainty region around the radiation energy, E_{rad} overlaps the uncertainty region around the peak energy, E_{peak} . The uncertainty region is $E_{\text{SigMult}} * \text{PeakEUnc}$ for the peak, and $E_{\text{SigMult}} * \text{RadEUnc}$ for the radiation. The E_{SigMult} is an uncertainty multiplier, its value is 4 by default. This search process gives a very broad list of matching radiations, purely by the energies.
- Calculating the 'spectroscopic strength' value, which is a normalized sum of the $\text{PeakInt} * \text{Efficiency}$ values. This gives a rough descriptive number about the presence about the important library lines for each component. If the spectroscopic strength is below a threshold value (10% by default), the component will be skipped from the further analysis.
- Peak merging: the algorithm now merges together the peaks whose distance is less than $\text{MaxFwhmContract} * \text{FWHM}$ channels (default $\text{MaxFwhmContract}=1.5$). This is because the identification is much more robust, if the unnecessarily splitted doublets are joined again, and their summed areas will be splitted by the nuclide identification algorithm.
- Determination of component clusters. If no overlapping peaks exist between two components, then their activities may be determined independently, thereby reducing

the computation time and increasing stability. Similarly, overlapping detection introduced for component clusters (a set of components), not just single components, which can be identified quantitatively in an independent way.

Fitting intensities of components

- If a peak is not found in the spectrum at the position of a library line, a virtual peak created. Its area assumed to be zero, while its area uncertainty is computed from the efficiency curve, the FWHM and the actual background under the missing peak. This way a missing peak is also takes part in the activity fit of the component.
- Together with the activity fitting, the correlation is also determined between the components of the cluster. If two component shares at least one spectrum peak, then they are correlated. If the correlation is very high, exceeding MaxCompCorr value (it is 0.99 by default), then we treat the two or more components non-distinguishable. An example would be two nuclei, both having only one significant gamma line at nearly the same energy. In this case, no independent activities may be calculated purely from the spectrum, by any means. In this case, we collect these highly-correlated components into component groups, and determine them together.
- Another fitting performed on the linear equation system, which tries to describe the measured spectrum peaks and also accounts for the background under the missing peaks.
- Checking if all of the spectrum peaks is well-described by the sum of the counts originating from the components' gamma lines. If there is significant difference between the peak area and the sum of library line intensities for a peak (significance threshold is 4 by default), then we re-fit the problem by allowing large discrepancy at that peak.

Final nuclide identification steps

- Checking the fitted activities of the components. In case unphysical values (zero or negative activities), dropping the component in question, and performing the fitting again.
- Filtering the final component list by the activity uncertainties: if that is higher than a threshold value (35% by default), then the components dropped, and a re-fit is performed. The components then sorted by the uncertainties of their activity values.

10. Batch spectrum evaluation

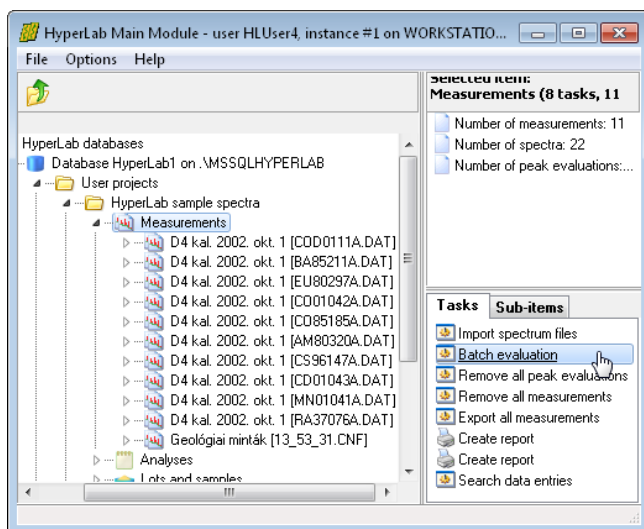
HyperLab provides more automatic spectrum evaluation tools, which are able to silently evaluate several measurements each after the other, with minimum user intervention. This makes it possible to perform the routine spectrum evaluation in a semi-automated way, and may speed up the work of the gamma spectroscopist.

10.1. Database batch evaluator

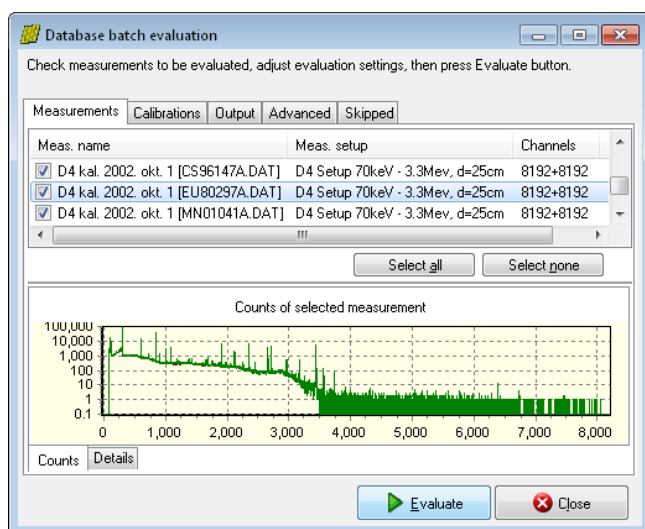
The database batch evaluator is a special peak evaluation tool of HyperLab Main Module. It is able to automatically evaluate several measurement entries stored in the database, each after the other.

10.1.1. Using of Database batch evaluator

To use the Database Batch Evaluator, open the project in Main Module where your spectra are stored.

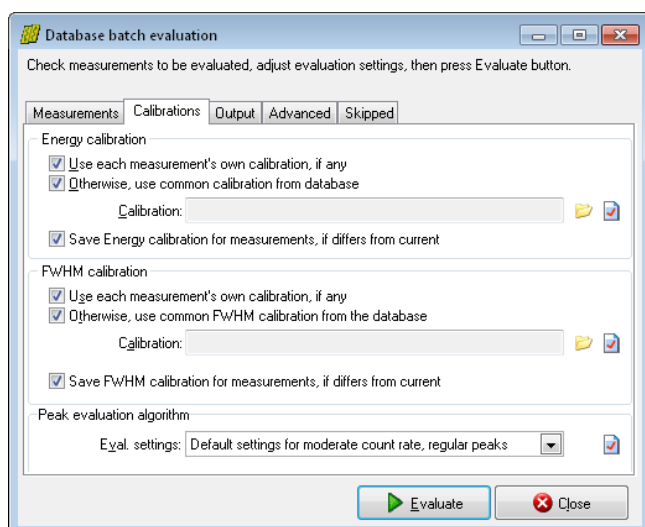


Click on *Measurements* node under the project, then select *Batch evaluation* task.



Now an evaluator window appears, listing all measurements assigned to this project.

Check the list if it is really required to evaluate all spectra. If a measurement is to be skipped, un-check it.



Change to *Calibrations* tab. Set the source of calibrations according to your measurement environment.

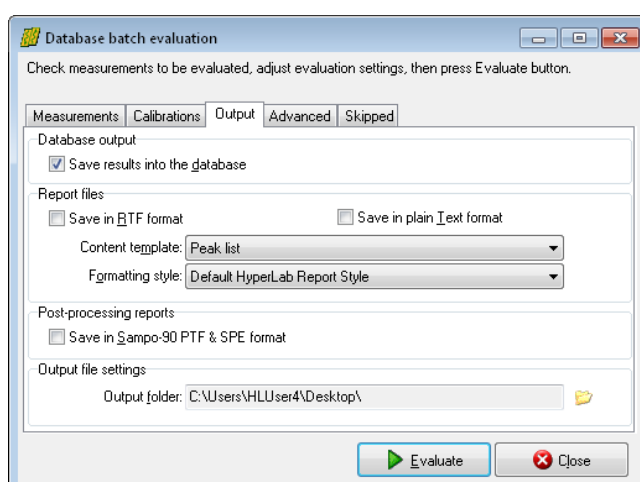
It is possible to use either the measurement's calibration or an arbitrary one from another measurement.

Specify evaluation output options under *Output* tab.

You can save results into the database; as well as generate textual reports or Sampo files for post-processing.

Do not forget to set the folder where your report files will be saved.

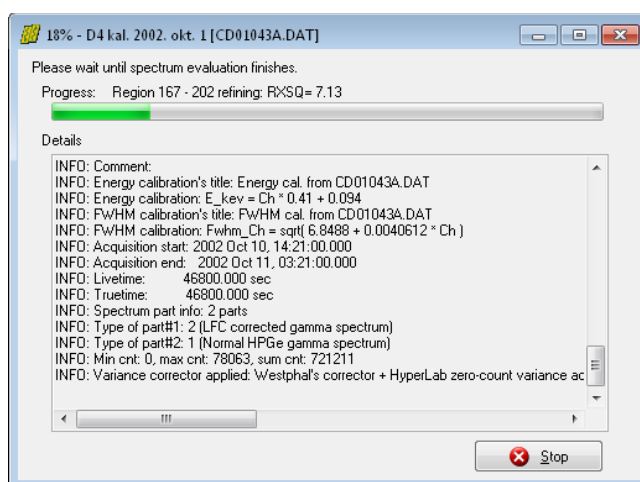
You may also specify some other settings under the *Advanced* tab.



Click the *Evaluate* button to initiate batch evaluations.

A new page appears now, displaying the overall progress of the batch as well as detailed messages for the last few measurement evaluation.

When evaluation finishes, press *Close*.



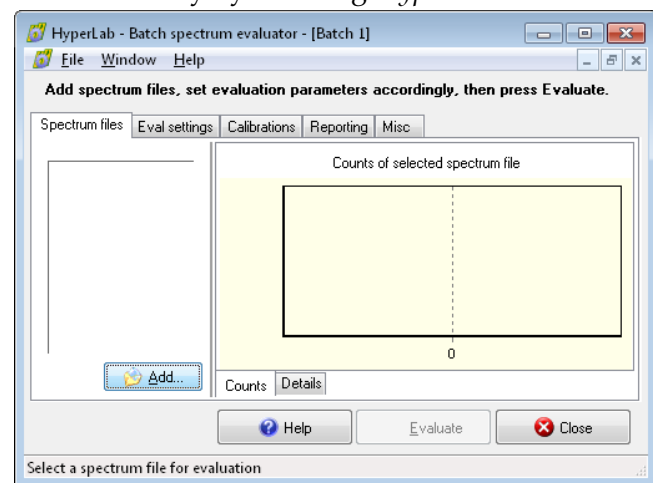
10.2. Spectrum file batch evaluator

The spectrum file batch evaluator is a standalone utility of the HyperLab System. It is capable of automatically evaluating more than one spectrum *files*, each after the other.

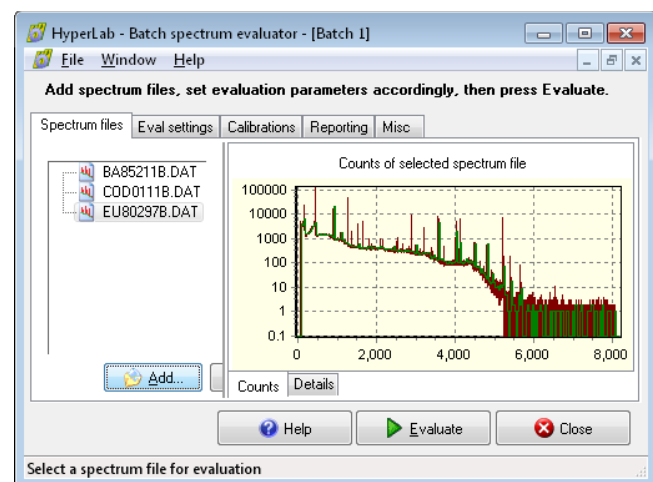
This utility does not require usage of HyperLab databases, as it operates on simple spectrum files, and its results are also saved into disk files. If you want to use batch evaluation for measurements stored in a HyperLab database, or you want to refine the fits manually, consider using Database batch evaluator instead.

10.2.1. Using of Spectrum file batch evaluator

Start the utility by selecting *HyperLab 2021 / Batch Evaluator 2021.1* from your Start menu.



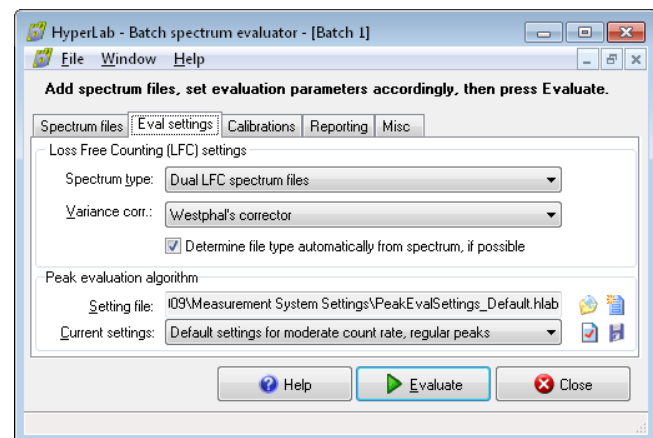
The evaluator dialog appears now.



Click on *Add...* button under Spectrum files tab.

A file open dialog appears now.

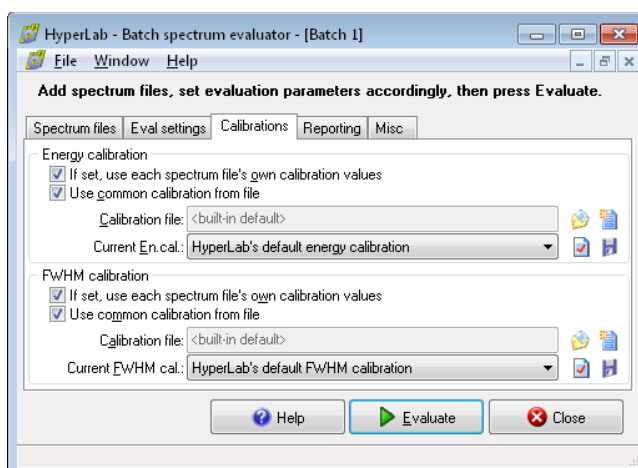
Select your spectrum files to be loaded, which will be listed at the left side of the utility.



Change settings under Eval settings tab.

Most important is to correctly set the type of spectra: '*Common gamma spectrum files*' or '*Dual LFC spectrum files*'.

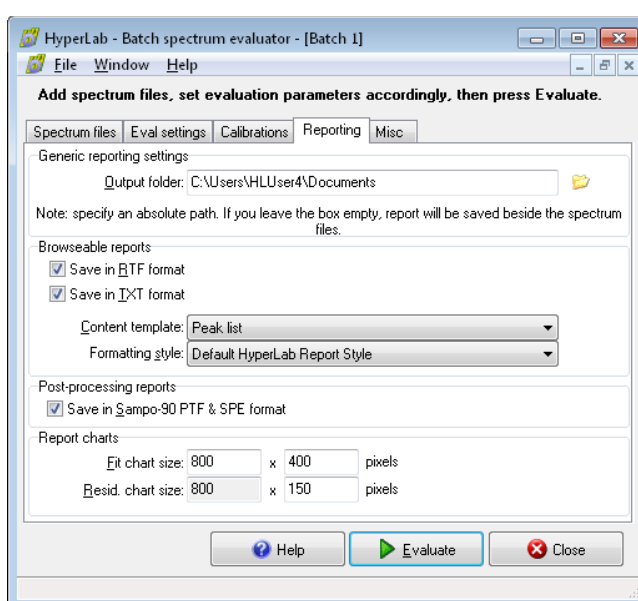
You can also set calibrations on Calibrations tab, if it is missing from the spectrum files. It is also possible to abandon spectrum files' calibration values, and import common energy and FWHM calibration values from text files.



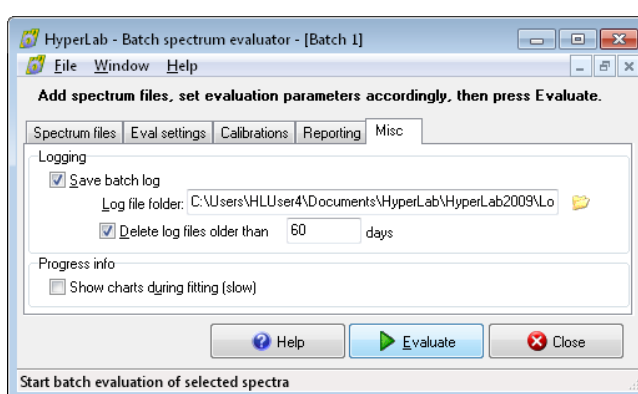
Set reporting options under Reporting tab. HyperLab is able to create reports in the following format:

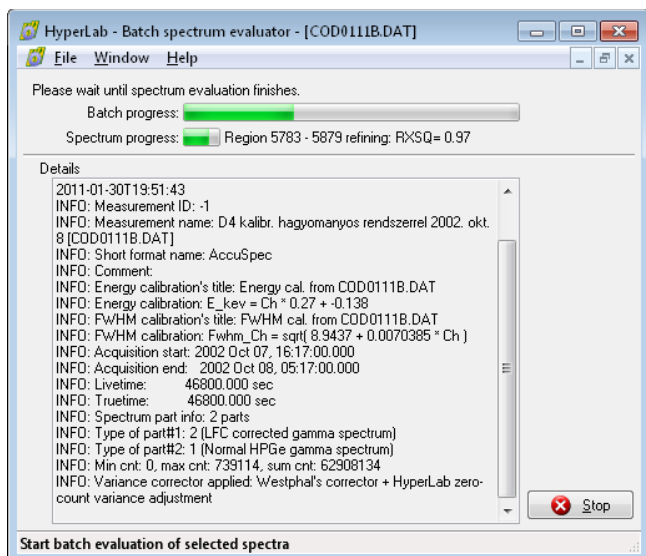
- Sampo-90 *.ptf and *.spe files
- Plain text files (*.txt), using HyperLab's report templates.
- Formatted Rich Text report files (*.rtf), using HyperLab's report templates.

Do not forget to set the output folder of your reports, otherwise the report files will be created into the folder of the spectrum files. HyperLab's report templates are contained in separate files, and can be edited, created, deleted by the user. Rich Text Files also may contain pictures of the fitted regions, revealing the fine details even for a batch evaluation. Please select an appropriate report template if you want to check your fits also with region pictures.



You can set miscellaneous options under Misc tab. You can set the folder of log files here, which is used by HyperLab when creating log files for the batch evaluation.





Press *Evaluate* button to start the batch.

HyperLab now evaluates all of the selected spectrum files, and creates report files as well as log files about them.

During evaluation, you can minimize the utility and work with other programs.

After the end of the batch, click *Close* to finish the evaluation.

11. Advanced database manipulation

Although HyperLab utilizes relational databases as primary data storage method, there is no need to interact with its raw data in the course of your daily work. There are cases, however, when an advanced user requires direct access to the data contained in HyperLab databases. As the following sections will contain several database diagrams, we provide a quick overview of database terminology and the database diagrams used within HyperLab documentation.

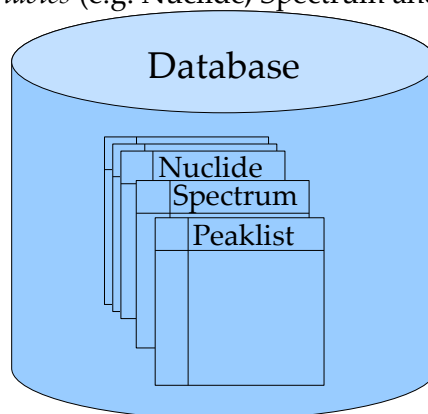
11.1. Database structure basics

Relational databases use a strict, well-defined hierarchy for data storage and retrieval.

Databases

The database is at the top level: it is a standalone entity encompassing all data that may be in connection to each other by any means.

Databases contain several *data tables* (e.g. Nuclide, Spectrum and Peaklist tables).



Data tables

Database tables consist of a header and *data rows*, and each row has exactly identical inner structure. Data rows are also called *records* in database terminology.

NUCLIDE_ID	A	Z	Symbol
51124	124	51	124Sb
51125	125	51	125Sb
52126	126	52	126Te
...

This figure contains a small part of the Nuclide table. Several data records are contained, and each row describes a unique Nuclide entity. Records may be queried, updated, inserted or deleted in a data table.

Data fields

A record comprises of several *fields*. All records in a table must have fields of identical name and data type. For example, a Nuclide record contains the following data fields:

Field name	Field value	Type of field value
NUCLIDE_ID	51124	integer
A	124	integer
Z	51	integer
Symbol	124Sb	string

The values of the data fields may be queried or updated individually in a record, if the record is identified by its primary key (see below), and the field is identified by its name.

Primary keys

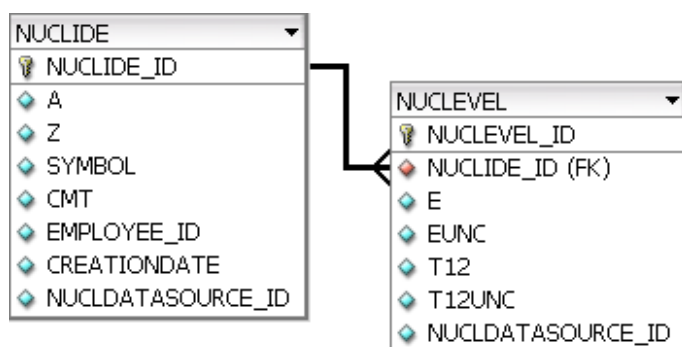
Database management systems are required to retrieve, insert and delete records efficiently. To accomplish this task, each record must be unique, that is, must be identified unequivocally within a table. For identification purposes, one or more field values are used together, thus forming an identifier, or *primary key*.

For example, unique identifier of the nuclide table is a special field named NUCLIDE_ID. As it is declared unique, the database management system guarantees that duplicated NUCLIDE_ID will never be kept in the Nuclide table.

Please note that the A, Z field combination also would have been used as a primary key, but a single primary key was chosen because of its simpler usage.

11.2. Database diagrams

Database diagrams provide information on database tables, fields, and logical relationships between tables.



The rectangular objects with heading depict *database tables*, where the heading contains the name of the table (e.g. "NUCLIDE").

The rows under the heading list the *data fields* in a specific table (e.g. "A" or "Z" means mass number and proton number for a specific nuclide).

The graphical symbol before the field name shows additional information about a field.



Regular data field.



Primary key data field; all primary keys together will uniquely identify the record.



Foreign key data field; references to a record of another table.

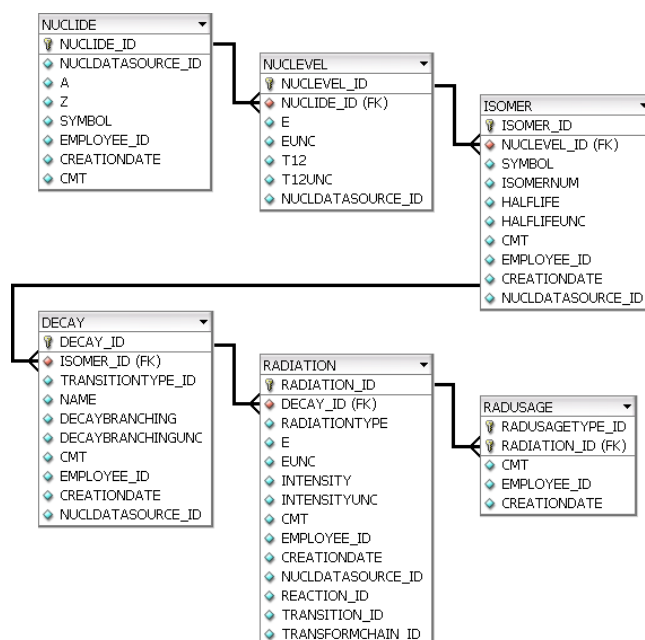


One-to-many relationship; depicts that many records of the second table may have reference to the same record of the first table.

In our example this means that more nuclear level entries may refer to the same nuclide.

11.3. Nuclear data structure in HyperLab databases

HyperLab databases contain nuclide, nuclear level, isomer, decay and radiation information.



For diagram legend, see section Database diagrams.

HyperLab's nuclear data tables are the following:

- Nuclide** Contains basic information about a nuclide (isotope). Its primary key is the NUCLIDE_ID, which is composed from the mass number and proton number.
E.g. nuclide with NUCLIDE_ID=51124 is 124Sb.
- NucLevel** Describes one nuclear level of a given nuclide. Contains level energy and lifetime information, and refers to its belonging nuclide.
E.g. level with NUCLEVEL_ID=511240002 is the E=10.86 keV level of 124Sb with HALFLIFE=93 sec.
- Isomer** Describes one specific isomer level (a nuclear level with practically significant life time). Contains a symbol for that isomer (e.g. "124Sb_m1"). Refers to the nuclear level which it belongs to. At most one isomer level may belong to a specific nuclide level.
E.g. ISOMER_ID=511241 refers to the isomer level of 93 sec mentioned before.
- Decay** Describes one decay which starts from an isomer level. Also contains a descriptive name for that decay, e.g. "124SB IT DECAY (93 S)". Zero, one or more decay may belong to a specific isomer.
E.g. DECAY_ID=5112410 is the isomer transition, and DECAY_ID=5112411 is the β^- decay, both originating from the same 93 sec isomer of 124Sbm1.
- Radiation** Describes one radiation for a decay (or for another nuclear event). Contains energy and intensity information, and refers to its parent decay.
E.g. RADIATION_ID="D05112411000001" is the 602.72 keV radiation of the 124Sbm1 isomer's β^- decay.
- RadUsage** This table contains radiation usage flags. One RadUsage record designates if a specific radiation may be used for a given task in HyperLab. Usage types include "Energy calibration", "Efficiency evaluation" etc. About their manipulation, see more details in Nuclear data library management.

11.4. Nuclear data library management

HyperLab inserts significant amount of nuclear data into each HyperLab database during the installation. This section describes the most important database editing tools regarding nuclear data. See also detailed information in section Nuclear data structure in HyperLab databases.

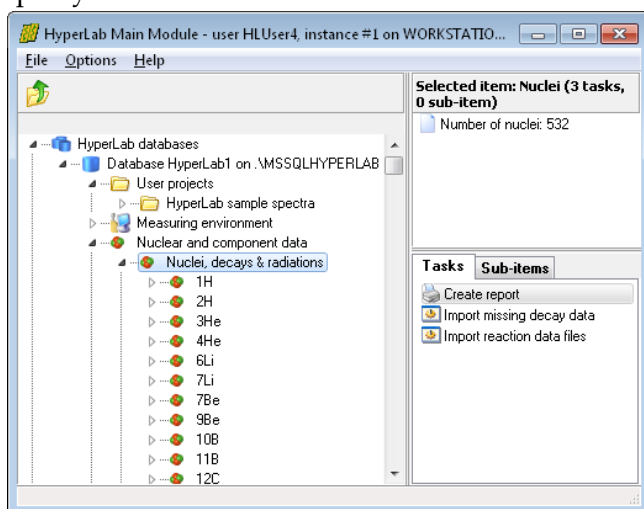
11.4.1. Editing radiation usage flags

HyperLab makes it possible for you to decide if a radiation may be used for a particular purpose, e.g. for energy calibration, efficiency determination and so on. This is achieved through the radiation usage flags, which can be conveniently edited on the given radiation's property page.

In our example we show a method that is applicable to permanently disable the 443keV lines of ^{152}Eu isotope for efficiency calibration purpose (these lines are improper for efficiency determination purposes because the level scheme results in two overlapping 443keV peaks).

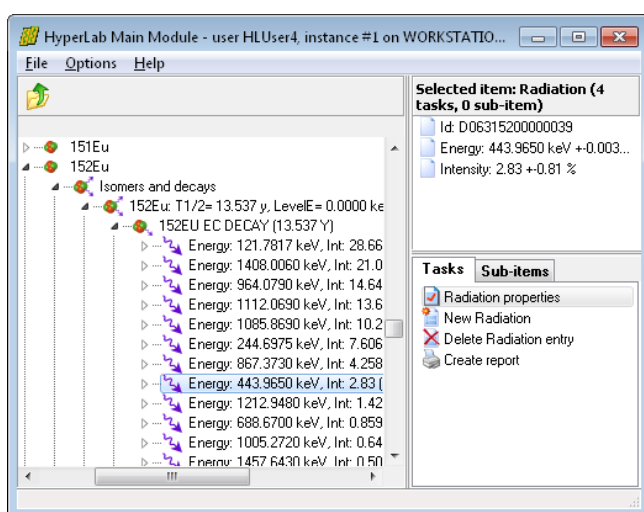
Locating the given radiation

Open your database in Main Module.



Double-click on *Nuclear and component data* node, then select *Nuclei, decays & radiations*. The list of nuclei is displayed now.

To quickly locate a given nuclide, click a nuclide node, e.g. " ^1H ", then quickly start typing the symbol of the searched isotope. In our case, type " 152 ". The data browser now locates the first nuclide with the typed mass number.



Double-click on ^{152}Eu node, then open its 13.5-year ^{152}Eu isomer and its ^{152}Eu EC decay.

If you check the list of radiations, you can observe the two 443-keV gamma lines of this EC decay. Click the first 443-keV radiation in the list, and select *Radiation properties* task at the right.

The radiation's property editor window appears now.

Editing radiation

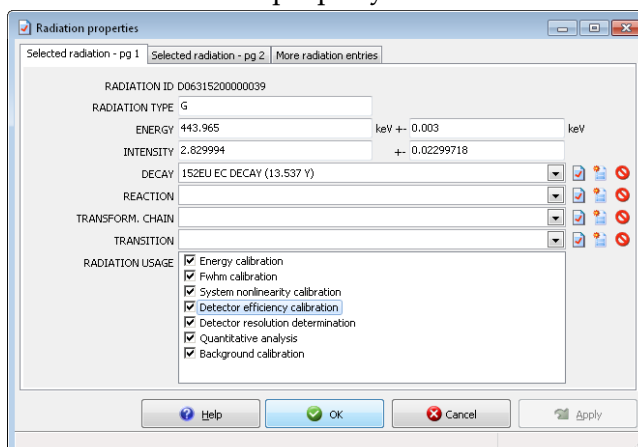
You can see the various usage types at the bottom of the radiation property editor window.

If a check mark can be seen beside a specific usage type, then this radiation will be used for that selected purpose.

Remove the check mark beside “*Detector efficiency calibration*”.

When you click this check box, the change will be immediately stored in the database, and next time the efficiency analysis module will not use this radiation.

Click OK, and repeat this editing for the other 443-keV line.



11.5. Importing data into external applications

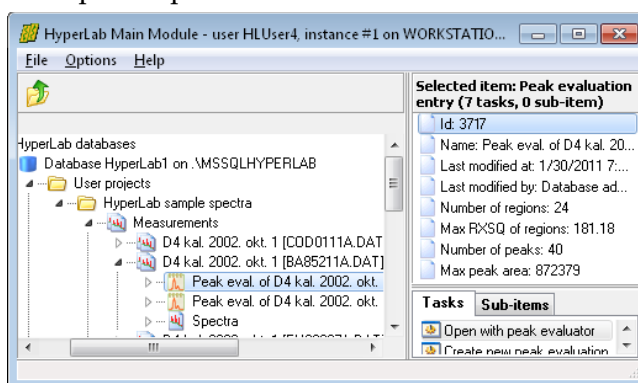
HyperLab databases contain all the data resulting from peak evaluations and various measurement system analyses. This section contains an example of the retrieval of such information. For newer Microsoft Excel versions you can immediately access the data, while other applications may require the creation of an ODBC data link for your database first. See “Creating an ODBC data source” for further details.

11.5.1. Importing peak lists

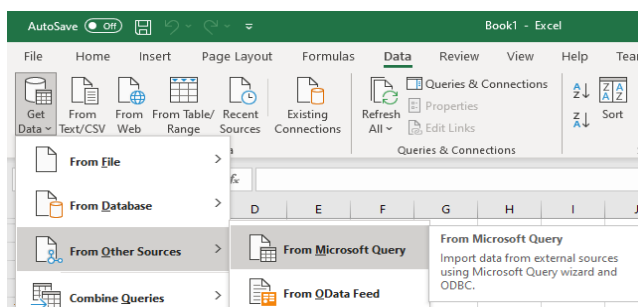
This example shows the importing the results of a specific peak evaluation into Microsoft Excel.

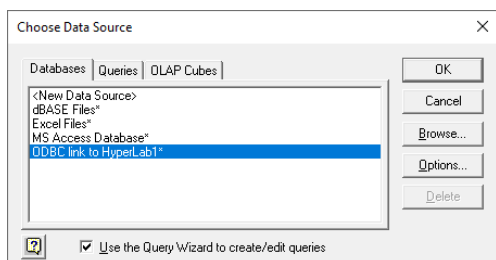
First you have to know the PEAKEVAL_ID number of the peak evaluation for which you want to query the evaluated peaks. You can find it as “Id” in the Detail lister window of the Main Module, when you click on the peak evaluation data node at the left.

In this case the Peak Evaluation Id is 3717.

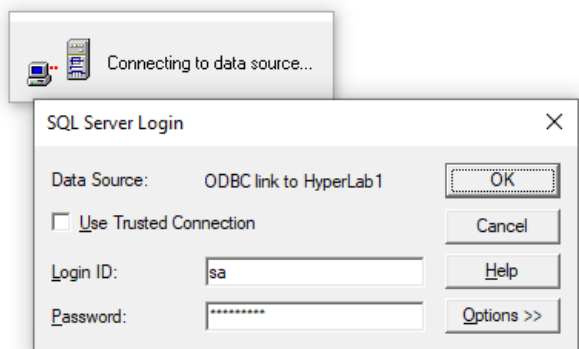


Start Microsoft Excel and select its *Data / Get Data / From Other Sources / From Microsoft Query* menu.

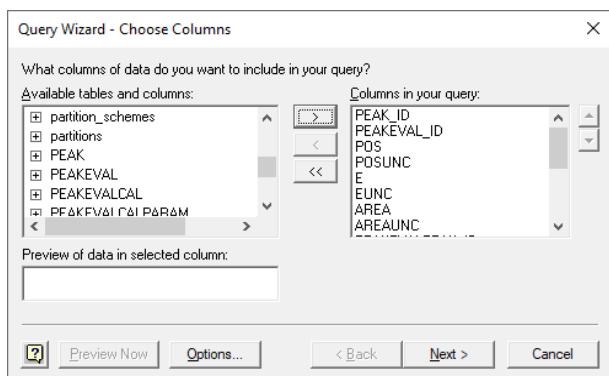




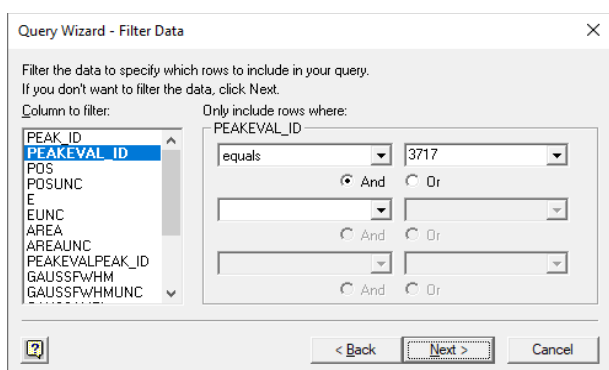
Select the ODBC alias you have created previously. Make sure that the *Query Wizard* check box is checked at the bottom, and click *OK*.



Microsoft Excel tries to connect to the database, and displays an SQL Server login dialog box. For default HyperLab installations, un-check the Trusted connection check box, and type your user name “sa” as well as the password. Default password for HyperLab 2021 product line is “Hlpwd2021” (in case of an upgrade, try hlpwd2002, hlpwd2005, hlpwd2008, hlpwd2009 or Hlpwd2014). Click *OK* when you are ready.



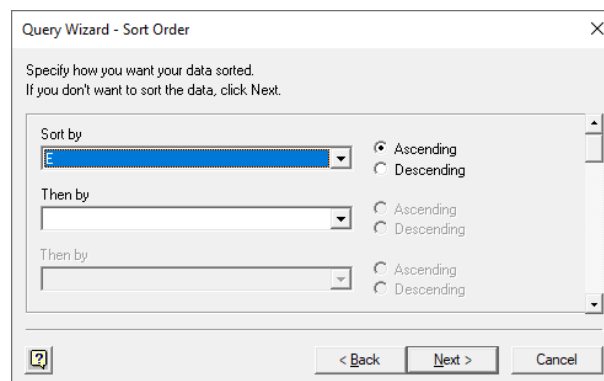
The Query Wizard appears now, where you can select the data table from which the data to be imported. Select *PEAK* table from the list of tables at the left, then click on the arrow button (“>”) pointing to the right, in order to add all fields of *PEAK* table to the list of queried fields. When you are ready, click *Next*.



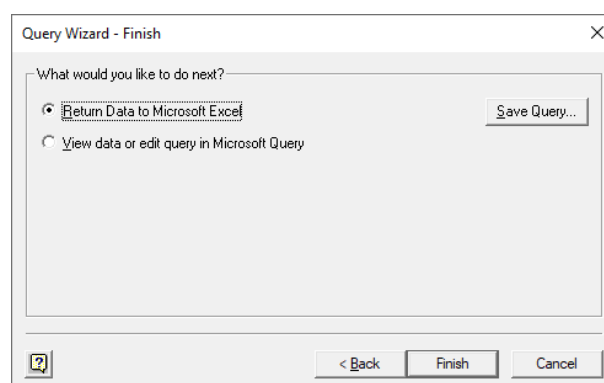
Now the *Filter Data* window appears. Here you can select a small subset of the records from the huge amount of peaks stored in the database. Filtering is performed via specifying a filter condition on the field values of the peak record. Only those peak records will be selected where this condition is met. In our case the condition requires that the peak evaluation of the peaks equals to 3717. To specify this condition, select *PEAKEVAL_ID* field on the left, “*equals*” operator at the

middle, and type in “3717” to the value field. When you are ready, click *Next*.

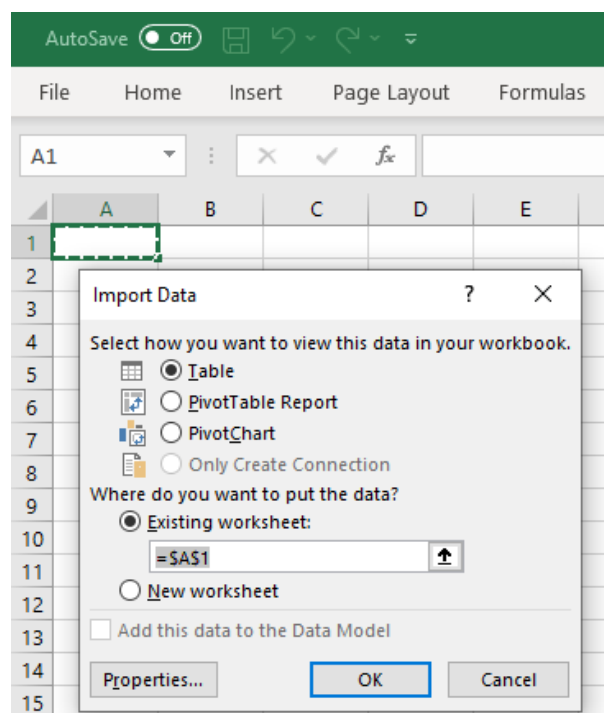
At the next step you can specify the sorting criteria. In our case it is advisable to select the energy field “E”, which sorts the peaks of a specific peak evaluation by their peak centroid. When you are ready, click *Next*.

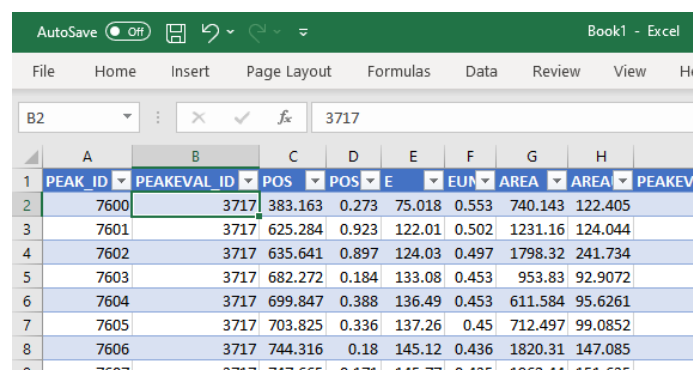


At the last step of the Query Wizard, simply click Finish button in order to return the queried data to Microsoft Excel.



Excel's worksheet displayed again, requiring you to specify a destination for the queried data. Specify the target location, and click *OK*.





	PEAK_ID	PEAKEVAL_ID	POS	POS_E	EUN	AREA	AREA	PEAKEV
2	7600	3717	383.163	0.273	75.018	0.553	740.143	122.405
3	7601	3717	625.284	0.923	122.01	0.502	1231.16	124.044
4	7602	3717	635.641	0.897	124.03	0.497	1798.32	241.734
5	7603	3717	682.272	0.184	133.08	0.453	953.83	92.9072
6	7604	3717	699.847	0.388	136.49	0.453	611.584	95.6261
7	7605	3717	703.825	0.336	137.26	0.45	712.497	99.0852
8	7606	3717	744.316	0.18	145.12	0.436	1820.31	147.085

Finally, the retrieved data is displayed in Excel, where further processing may be performed on it.

12. Database maintenance

The following sections describe the common tasks regarding HyperLab databases.

Generic information

HyperLab installs the Microsoft SQL Server database management software component by default.

HyperLab databases are kept in disk files, containing all measurement and evaluation information used by the spectroscopist. These database files are installed in your “Documents \ HyperLab \ Databases” folder by default.

These are the data files which contain your data, and you need a continuously running server application, which provides these data in a structured manner to every application that requires them. This is Microsoft's SQL Server, which is installed as a service application. These service applications are started automatically by Windows upon the boot process, even if no user is logged in to the computer. This way a properly installed and configured SQL Server application is ready to serve remote requests when the computer is switched on, so no special actions are needed on computers which are used as a central HyperLab database server.

12.1. Database creation

It is necessary to create new HyperLab databases when

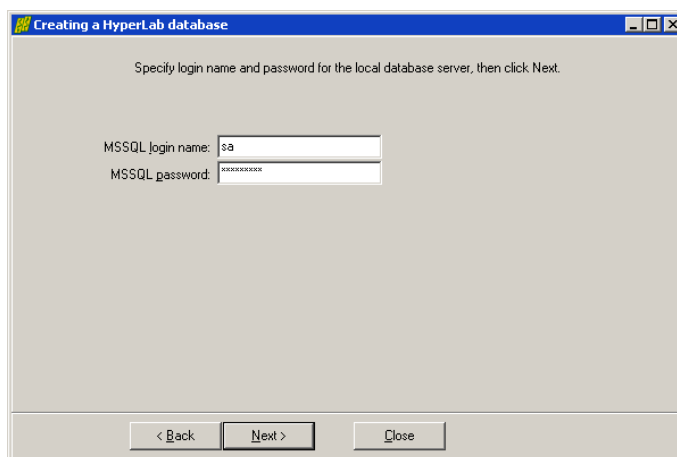
- you start using HyperLab, or
- it is advisable to separate measurement and evaluation information into two or more independent databases. This latter scenario is used e.g. when two spectroscopists work independently of each other, and keep their work separately; or when an institute working on two unrelated research fields.

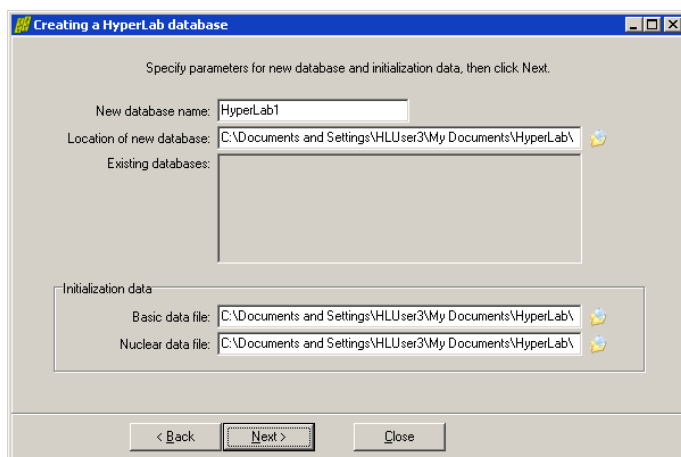
To create a new HyperLab database, follow the instructions below.

Click *Local database server* node, then on the task *Create a database*. Database creating wizard appears now. Enter login name **sa** and password for the database administrator.

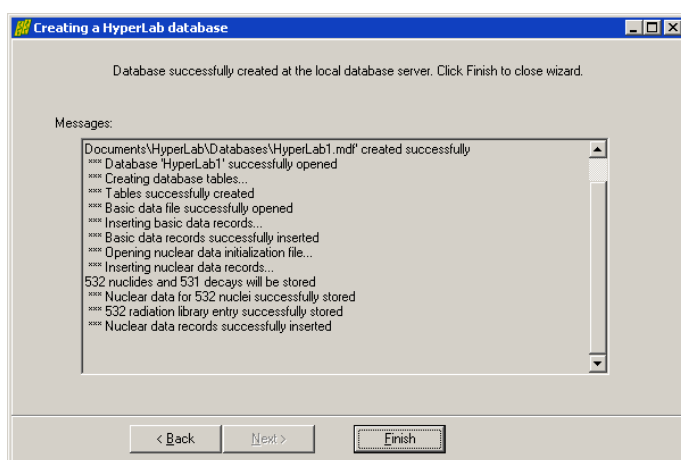
Note: Default database server password is **h1pwd2021** for the HyperLab 2021 product line (after an upgrade, you may also try **h1pwd2002**, **h1pwd2005**, **h1pwd2008**, **h1pwd2009**, **h1pwd2013**, **h1pwd2021**).

When you are ready, click *Next*.





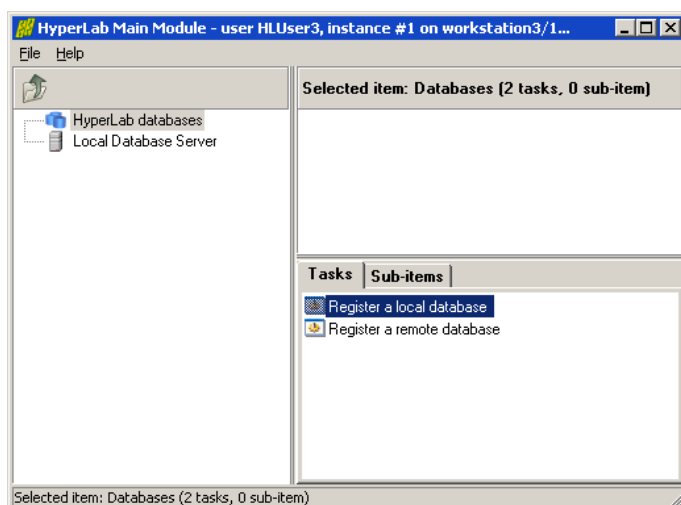
Specify the name of the new database, then click *Next*.



An automatic database creation process is started, which also incorporates the copying of large amount of nuclear data to the new database. The process may take several minutes. When the copying process ends, click *Finish*.

12.2. Database registration

When you create a new HyperLab database, SQL database server will be its owner. However, sometimes HyperLab will not be aware of this new database without *registering* it. During registration, an entry is created in the file *Documents \ HyperLab \ HyperLab2021 \ RegisteredDatabases.xml*, which will direct HyperLab to display the database in the Main Module's database browser tree, under *HyperLab databases* node. In order to register a newly created local database, follow the steps detailed below.



Click on the *HyperLab databases* root node in the database browser tree of the Main Module, then click *Register a local database* task from the Tasks window.

The local database registering wizard appears now. Enter a valid database user name and password, then click *Next*.

The screenshot shows a window titled "Registering a local HyperLab database". The instruction text says: "Specify login name and password for the local database server, then click Next." There are two input fields: "MSSQL login name:" with the text "sa" entered, and "MSSQL password:" which is empty. At the bottom, there are three buttons: "< Back", "Next >", and "Close".

Select a local database that is not currently registered, then click *Next*.

The screenshot shows the same window titled "Registering a local HyperLab database". The instruction text says: "Specify database name, then click Next." There is a dropdown menu labeled "Database name:" with "HyperLab1" selected. At the bottom, there are three buttons: "< Back", "Next >", and "Close".

If the selected database is accessible on the local database server, you can specify a description for the database. This description will be displayed in Main Module's database browser tree, under *HyperLab databases* node. Also some attributes of the local database server are displayed.

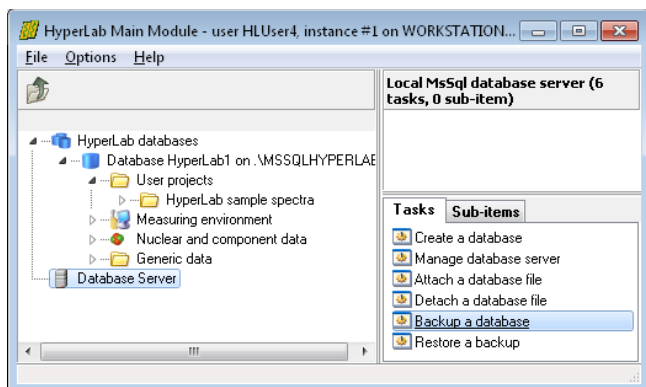
When you are ready, click *Finish*.

The screenshot shows the same window titled "Registering a local HyperLab database". The instruction text says: "Local database successfully connected. Please change its description, if needed, then click Finish to register it." There is a text input field labeled "Description:" with the text "HyperLab1 database on local machine" entered. Below it is a section labeled "Additional info:" containing a list box with the following text: "Database name: HyperLab1", "Database server: WORKSTATION3", "Database server version: 8.00.760", "Database server level: SP3", "Database server edition: Desktop Engine", and "Database server collation: SQL_Latin1_General_CP1_CI_AS". At the bottom, there are three buttons: "< Back", "Next >", and "Finish".

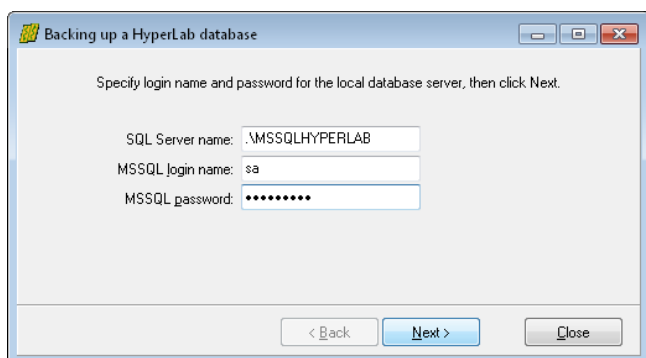
12.3. Database backup

Regular backup of your working environment is essential if you want to avoid a dreaded data loss accident. Fortunately, as HyperLab stores every important piece of information in a database, this is reduced to just two simple steps:

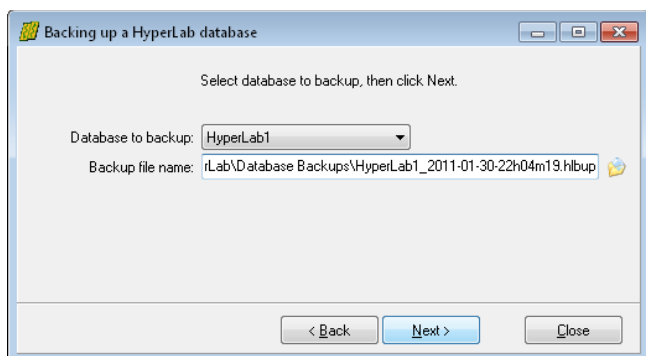
- back up the database,
- move the single backup file to a safe location. This should not be on the same computer.



To initiate a backup, select *Database Server* item on the left, then click the task *Backup a database* on the Tasks pane.



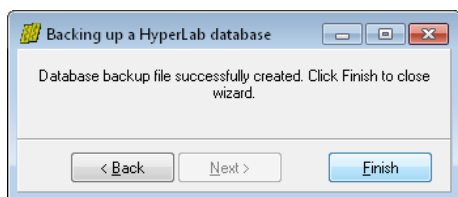
Specify database user name and password, and click *Next*.



Select the database to backup. In this example, we have chosen the *HyperLab1* database.

The name of the backup file is automatically generated, so you do not have to modify it.

If you are ready, click *Next*.



Now the backup operation starts.

It should finish within a few minutes for even moderately sized databases.

After backup ended, a message appears in the backup window. Click *Finish* to acknowledge it.

! Do not forget to copy your database backup file to a safe place (e.g. to a DVD) !
Do it immediately after you performed a backup, otherwise your data may be lost in case of a computer failure.

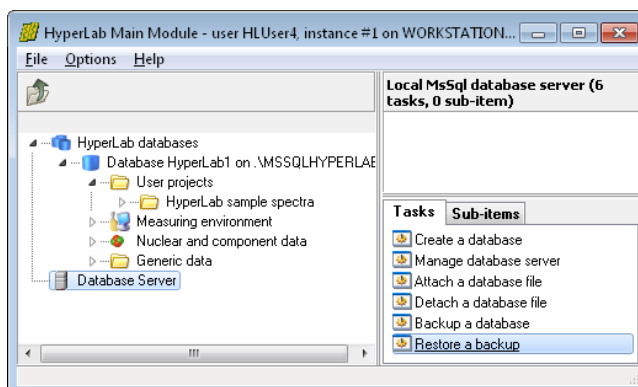
12.4. Restoring a database from backup

Database backup files has essentially two usage in case of HyperLab:

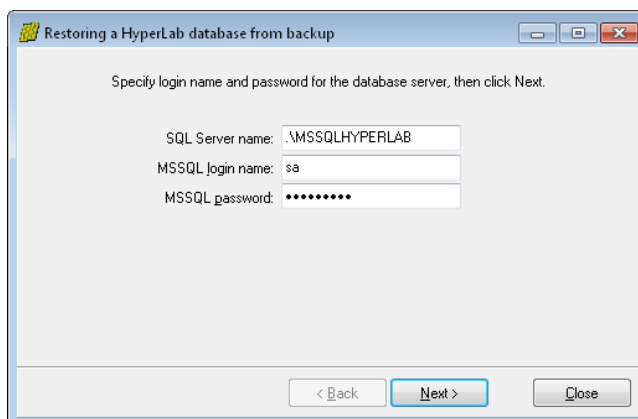
- Protect your precious measurement and evaluation data against being destroyed,
- Provide a simple mean to transfer your complete work from one workplace to another.

The process of taking a previously created HyperLab backup file, and turn it back to a usable database called *Restore*.

To initiate a database restore, select *Database Server* item on the left, the click the task *Restore a backup* on the Tasks pane.



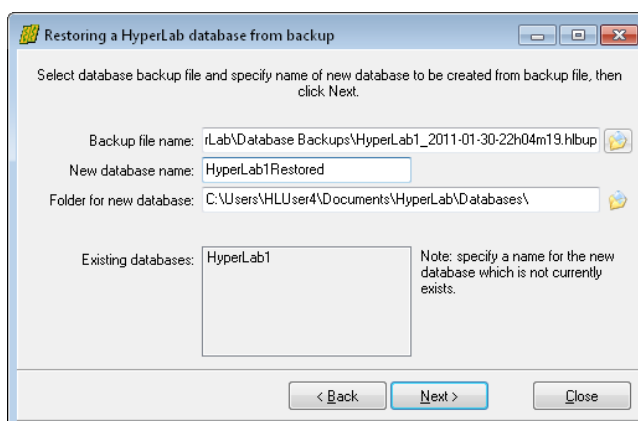
Specify database user name and password, and click *Next*.



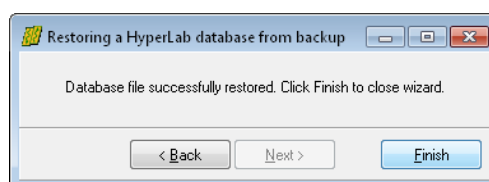
Select the backup file by clicking on the folder icon at the right.

The *New database name* contains the name of the database that will be created from that backup file. You are not allowed to specify an existing database, otherwise it would be overwritten.

If you are satisfied with the restore parameters, click *Next*.



After acknowledging an information window, restore process starts. Finally a dialog appears, showing the status of the restore operation. Click Finish to close the window. After you registered the new database in your HyperLab application, you can start using it.

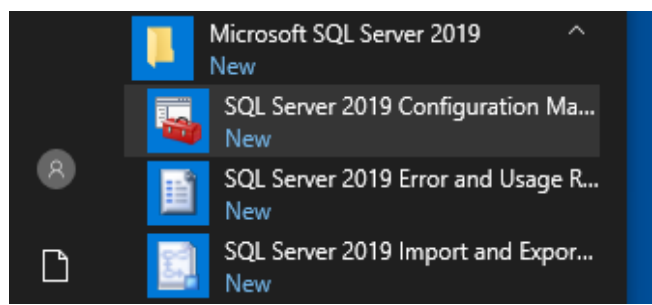


12.5. Configuring remote access

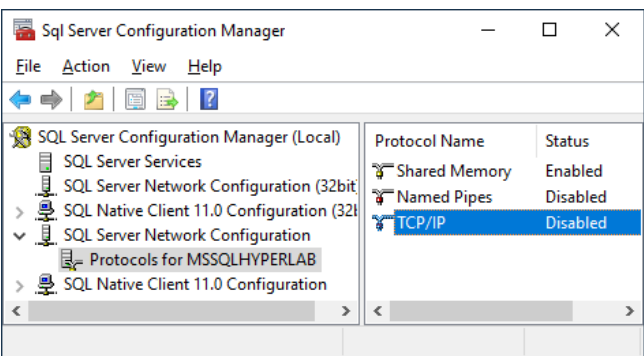
Please note that a newly installed SQL database server will not be accessible from the network unless you enable TCP/IP networking protocol for the SQL Server application. This is due to security reasons: virtually every remotely accessible service may lead to a system compromise. **Note:** If you are using a database only from the same computer – in other words, you are using 'Local database' topology – you *should not* enable remote connections.

Enabling TCP/IP networking protocol for the SQL Server

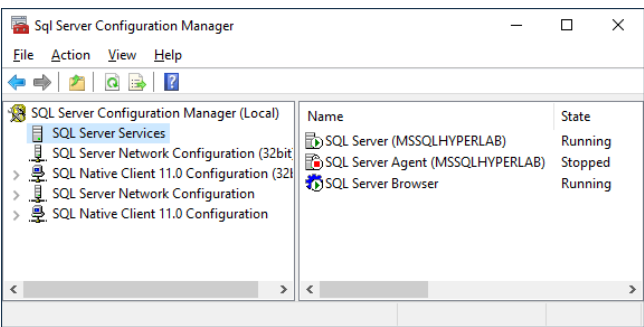
If you want to enable remote HyperLab Main Module instances to connect to you database server, enable its TCP/IP networking protocol by performing the following steps:



Please start SQL Server Configuration Manager manually from the start menu to configure network protocols. Start this utility by click on Start / Microsoft SQL Server 2019 / SQL Server 2019 Configuration Manager shortcut. This requires Administrator privileges.



When the configuration utility starts, open the *SQL Server Network Configuration* node on the left, then click on *Protocols for MSSQLHYPERLAB* item. Check at the right if the status of the *TCP/IP* is *Enabled*. If this is the case, then the database server is accessible from other computers via TCP/IP networking, so you can skip the further steps.



If the status is Disabled, then right-click on it, and select Enable. A message will pop up, notifying you about that an SQL Server restart is required to the changes coming into effect. To restart SQL Server, click SQL Server Services at the left, then right-click over SQL Server (MSSQLHYPERLAB) on the right. Choose Restart from the popup menu, and wait until it completes.

You can access your HyperLab databases from other computers now.

Enabling communication through firewalls

As a networked SQL Server accepts TCP/IP requests through the network, it requires appropriate network ports opened on your firewall. For default installations, the **TCP port 1433** should be enabled.

Note: Opening a port on your firewall poses severe threat to your computer system. Open the port only for the computers on your LAN, and only if remote access is really required. See <http://support.microsoft.com/kb/841252> for details.

12.6. Database upgrade

The inner structure of the HyperLab databases is rarely changing with newer versions of HyperLab, and these minor changes are transparent for different HyperLab versions – that is, the HyperLab 2002, 2005, 2008 and 2009 branches are able to use the same databases.

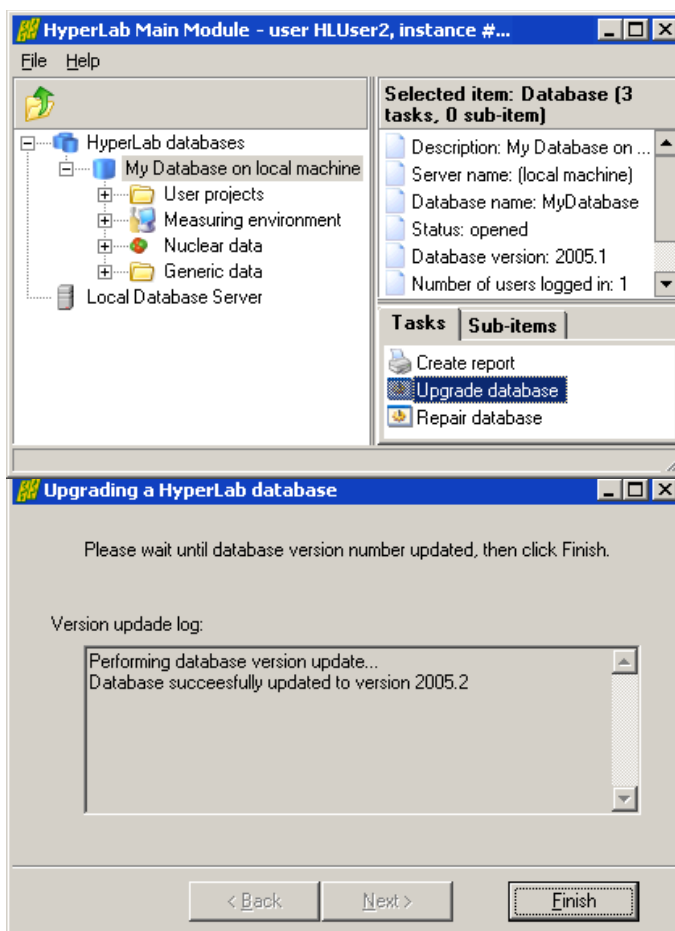
However, from HyperLab 2009, advanced database functions are introduced. These new functions of HyperLab require at least the 2009.1 version database.

Several bug fixes and serious *speed enhancements* (e.g. significantly shorter saving times in peak evaluation module) are also incorporated in the 2005 or 2008 version of databases, so it is always advisable to upgrade at least to this format.

You are not required to create a new database in order to utilize these new functions, as HyperLab Main Module provides you with a Database Upgrade tool, which is capable of performing these changes in-place.

To upgrade your database to a newer version, please follow the steps below:

1. Always create a backup of your database before the upgrade. This way you will not suffer any data loss should the backup operation fail.
2. Start HyperLab, and open the database you want to upgrade. Please note that the version of the database is displayed at the right panel.
3. Select *Upgrade database* task. A wizard page appears now. The upgrade information panel contains the possible upgrade steps. Click *Next*.
4. Please wait while the database upgrade is in progress, then click *Next*, and *Finish* on next page. When you open your database next time, it will correctly indicate the new version number.



12.7. Moving databases between computers

HyperLab makes it possible to transfer all your data in your databases from one computer to another. There are plans to implement an export – import utility, which will be able to transfer standalone data items between databases, but it is not implemented yet: only complete databases may be transferred.

There are basically two methods for transferring databases between computers:

- **Backup** the database and restore it on another computer. This way one single backup file is created, which can be easily transferred to another computer where it is restored as a new database. This is the preferred method.
- **Detach** and attach database files from the local database server. This method makes it possible to make a copy of the *.MDF (data) and *.LDF (log) files of the database and transfer it to another SQL Server. Use this method only if backup fails.

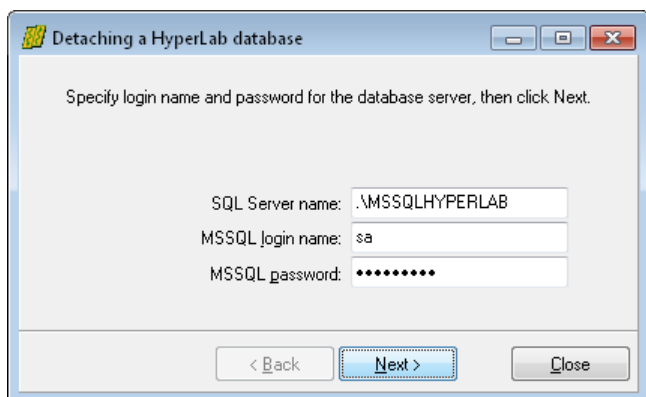
12.8. Detaching and attaching databases

When a database is used by SQL database server, it is locked: you are not able to even view into it, nor make a copy of it. This is due to data protection reasons. Detach operation will break the link between the database server and data files, while attach will rebuild this link again.

Detaching database files

You can detach a database from the database server, and this way it will stop using it. Now you can make an exact copy of the database, or delete the database files, if these become unnecessary.

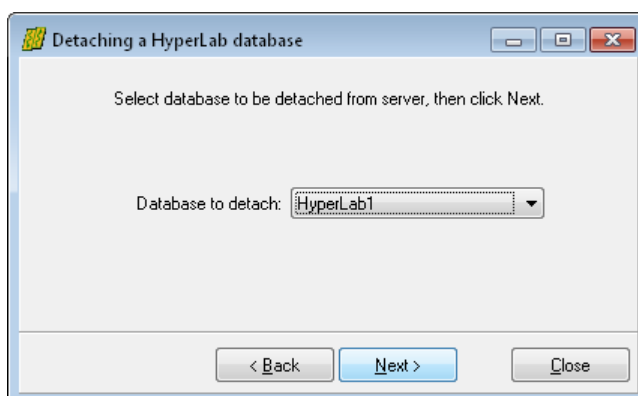
1. To detach a database from the server, click Local Database Server icon at the left, then select Detach a database file task from the right.



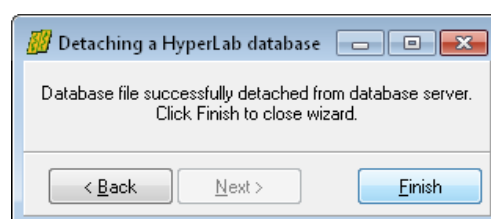
2. A detach wizard appears. Enter 'sa' database administrator name and your password to local database server, then click *Next*.

Note: Default database server password is **H1pwd2021** for the HyperLab 2021 product line (after an upgrade, you may also try h1pwd2002, h1pwd2005, h1pwd2008, h1pwd2009, H1pwd2013 or H1pwd2014).

3. A database selection page appears now. Select the database you want to detach, then click *Next*.



4. Click Finish to close the wizard.

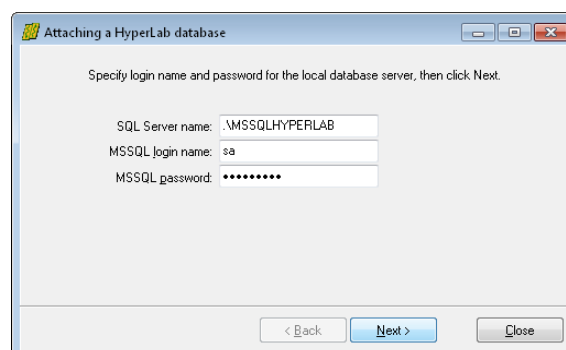


Attaching database files

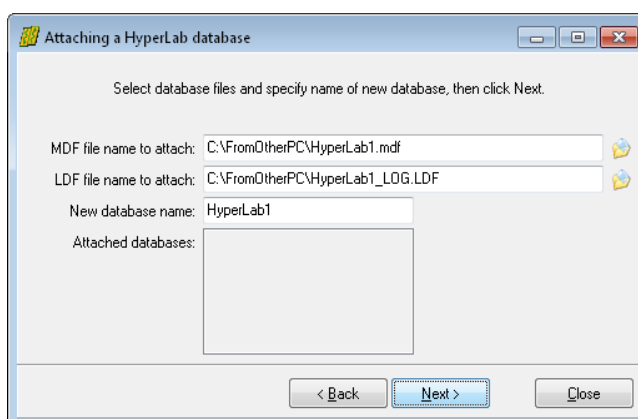
If you have a previously saved data file – log file pair, you can attach them to your local database server. After attaching, the server always search them at the specified location. Therefore, it is not advisable to attach files residing on removable media, e.g. on a USB key or a network drive.

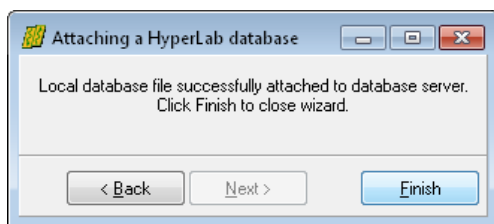
To attach a database to the SQL database server, click Local Database Server icon at the left, then select 'Attach a database file' task from the right. A detach wizard appears. Enter 'sa' database administrator name and your password to local database server.

Note: Default database server password is 'hlpwd2021' for HyperLab 2021 product line (in case of an upgrade, you may also try hlpwd2002, hlpwd2005, hlpwd2008, hlpwd2009, Hlpwd2013 or Hlpwd2014). If you are ready, click Next.



A database file selection page appears now. When you successfully selected the MDF file, the wizard will automatically fill up the LOG file name field as well as the descriptive database name. Change the LOG file name if it does not match your real file name. You can also modify the descriptive database name. When you are ready, click Next.





Now the attach process starts.

If an error message pops up about that the SQL Server has no right to access to the specified directory, then you should add Full access right to the predefined *NETWORK SERVICE* user over the folder and its content. Click Finish to close the wizard.

12.9. Creating an ODBC data source

Note: this step describes a fail-safe way to connect *any* third-party application to your HyperLab database. This step is not necessary anymore if you want to use solely Microsoft Excel for this purpose, because in recent releases it is able to directly access SQL Server databases.

ODBC data sources or data links are just a set of parameters stored in Windows. Various applications use these parameter sets to connect to a local or remote database.

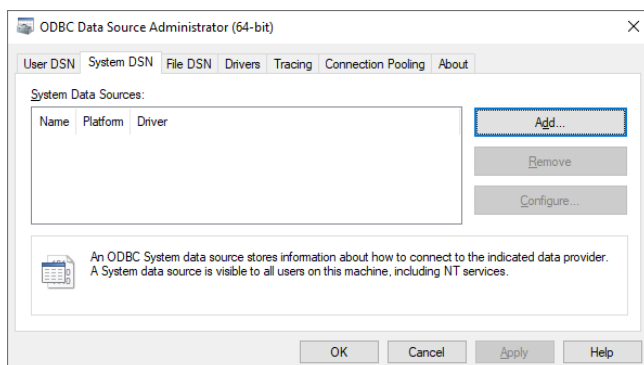
Newer HyperLab versions does *not* require the creation of an ODBC link to HyperLab databases (as opposed to HyperLab version 2002).

This section contains the detailed steps necessary to create an ODBC data source for a specific HyperLab database.



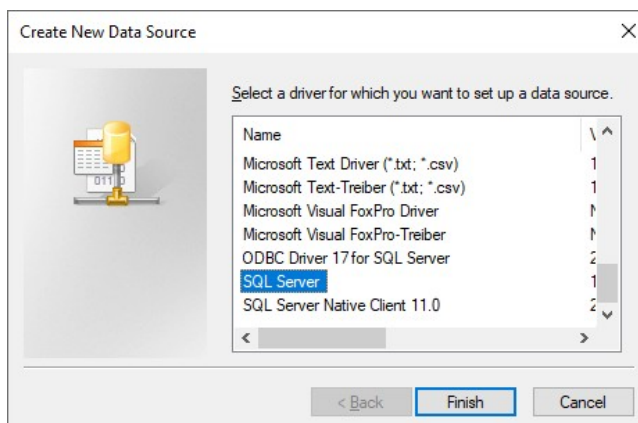
Open your Start menu, and start typing ODBC, then click on the *ODBC Data Sources (64-bit)* icon. Alternatively, open the old-style Control Panel, go to *System and Security / Administrative Tools*, then double-click the *ODBC Data Sources (64-bit)* icon.

Note: If you are using a 32-bit third-party application which wants to access a HyperLab database (like the older version of Microsoft Excel), perform these ODBC link creation steps with *ODBC Data Sources (32-bit)* instead.



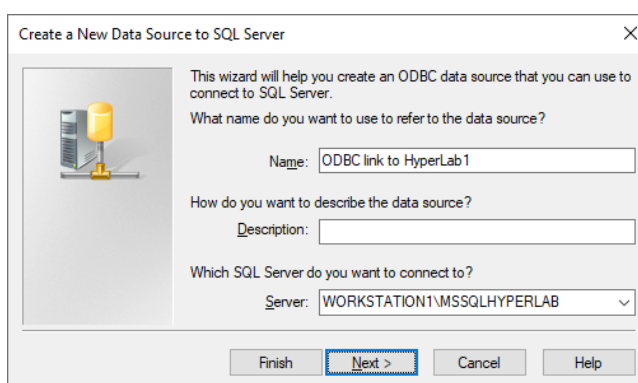
The *ODBC Data Source Administrator* window appears now. Click on its *System DSN* tab, and then on the *Add* button.

A database driver selection window appears now. Select the *SQL Server* item, then click *Finish*.



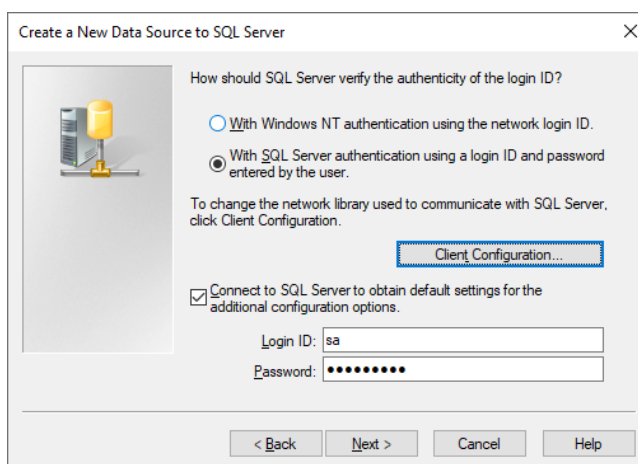
Specify the basic parameters of the new database link: give it a name and specify the SQL server. Server name is required in *ComputerName \ MSSQLHYPERLAB* format. Description field may be omitted. Click *Next* if you are ready.

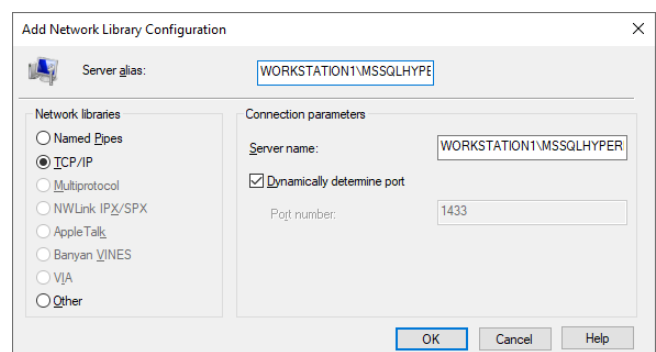
Note: If you are still using MSDE database server version (from HyperLab 2002 or 2005), you have to specify only the computer name. In this case type a dot (".") into the Server box.



A client configuration window appears now. Select the *SQL Server authentication* method, and type "sa" as user name to log in into the server, as well as the database password. Default password is "H1pwd2021" (in case of an upgrade, you may also try h1pwd2002, h1pwd2005, h1pwd2008, h1pwd2009, H1pwd2013 or H1pwd2014).

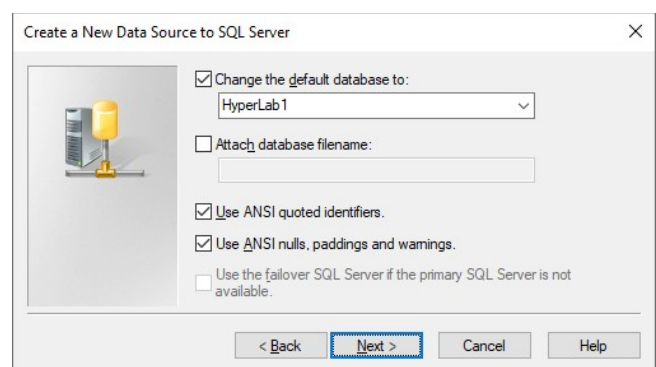
Finally click *Client configuration* button for detailed connection parameters.



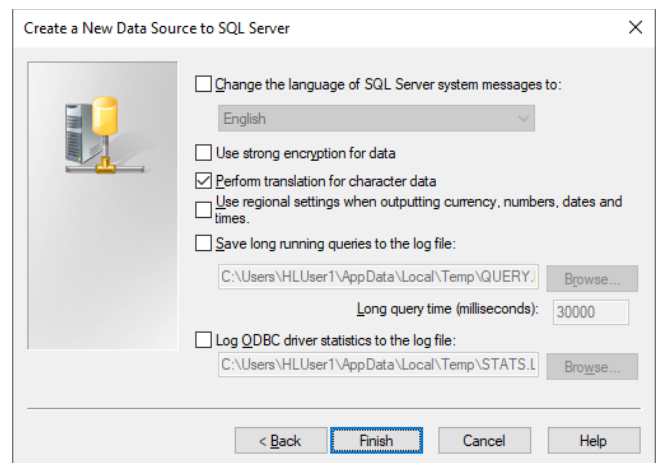


The *Client configuration* window appears now. Select TCP/IP network library. Please note that in order to make TCP/IP connection work TCP/IP network library must be enabled. See details in section “Configuring remote access” on enabling this. Click *OK* when you are ready.

The *Client configuration window* appears again. Click *Next*.



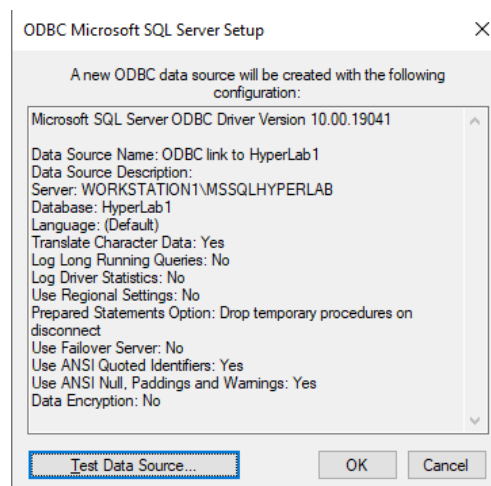
Place a tick mark beside check box “Change the default database to”, and select your SQL Server database from the drop-down list, then click *Next*.



Another database connection option window appears now. Change values if required, then click *Finish*.

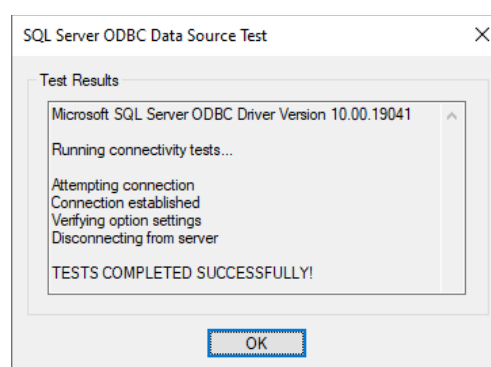
A summary page appears now, informing you about the ODBC alias created.

As it provides a testing facility, click *Test Data Source* button to initiate the testing of the newly created ODBC link.



A message box appears now, and provides basic information on the ODBC link status. If the “Test completed successfully” message appears here, your ODBC data source is ready to use by an external application.

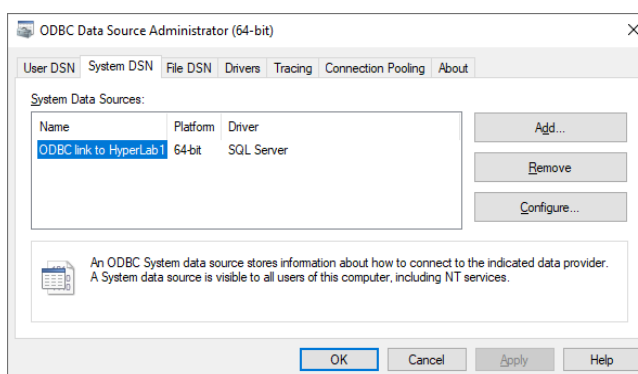
Click OK to close this window, and click OK again to close the summary page.



The *ODBC Data Source Administrator* window appears again, but now its System Data Sources list contains the new ODBC data link entry.

Click OK to close this window.

Now ordinary third party applications are able to access your HyperLab database. This way e.g. complex evaluations, say, a 64-bit Microsoft Excel-based activity calculation application can be developed.



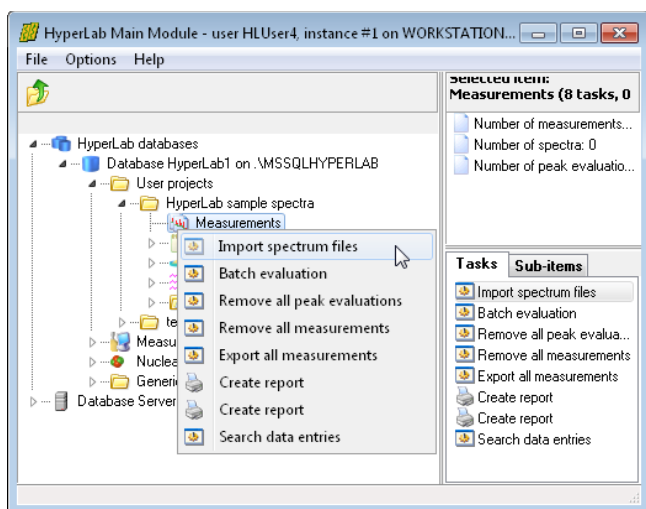
13. Importing sample spectra

In order to perform a sample nonlinearity, efficiency and resolution analysis, HyperLab provides some sample spectra. These should be imported to HyperLab database before performing any of these analyses.

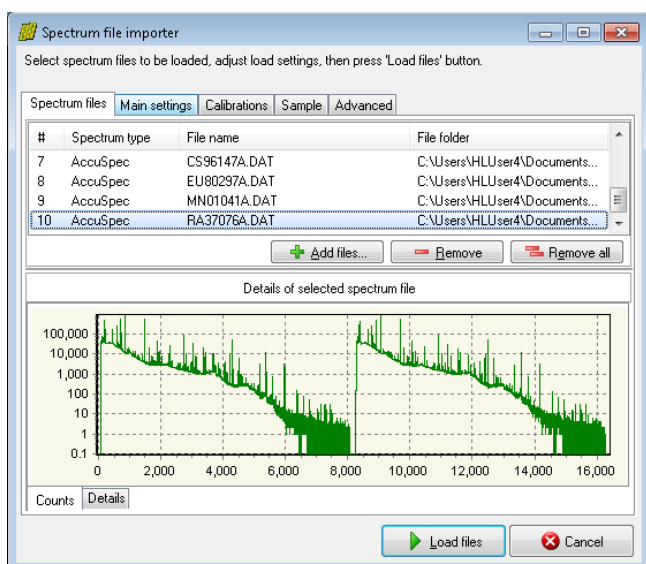
HyperLab arrives with sample sets for two measurement systems. These are assembled from the same devices, but using different energy ranges. Our description will only deal with HyperLab's sample spectra set for the system of 70 keV - 3300 keV range.

13.1. Importing steps

First create a project node in Main Module, which will contain all the sample measurements and their evaluations.



Then initiate the import of the sample spectra by right-clicking the *Measurements* node under the project and the select *Import spectrum files* from the pop-up menu.



Spectrum file importer window appears now.

Click *Add files* button, and select 10 sample Accuspec spectra with "A" ending in their file name, as can be seen in the picture.

Do not forget to check the settings under the *Main settings* tab.

Here you should specify the *Dual LFC* spectrum evaluation mode first, as these measurements are created using an LFC module, allowing compensation for count losses due to varying or high count rate situations.

At the *Measurement setup* combo box, you should select HyperLab's sample measurement setup. This is an important setting, because all calibration analyses, e.g. the nonlinearity will belong to a specific setup, thus the calibration assignment can be automatic.

If the sample setup can not be found in the list, create it by clicking on the *New entry* button beside the combo box.

If creating of a new measurement setup is necessary, this entry editor will pop up. The editing can be done on the regular way, as described in the *Importing spectrum files* section of the *Main Module Quick Start Guide*.

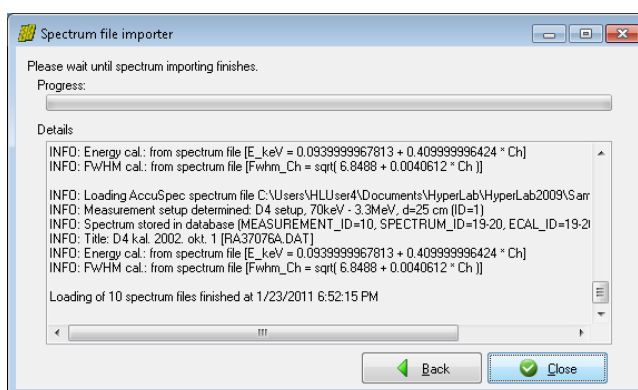
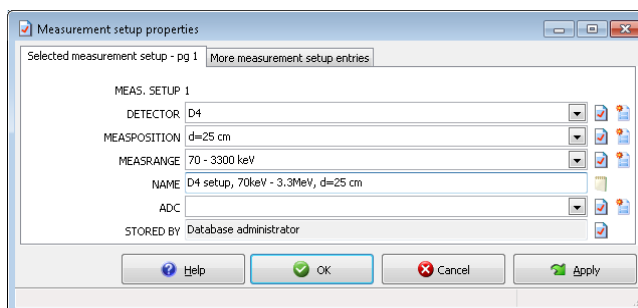
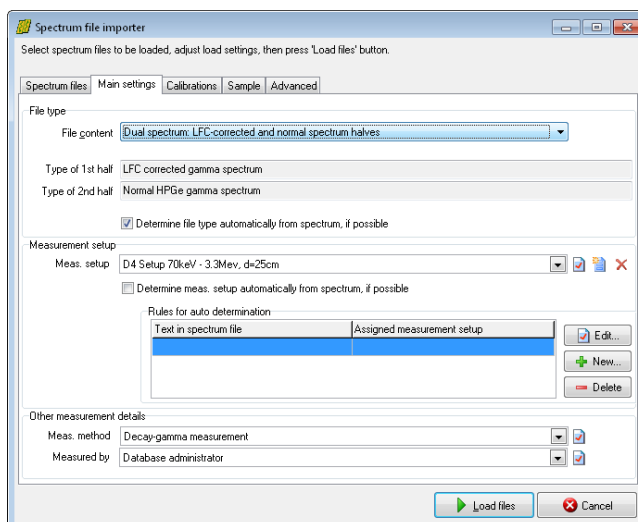
When you are ready, click OK. The spectrum import form will appear again.

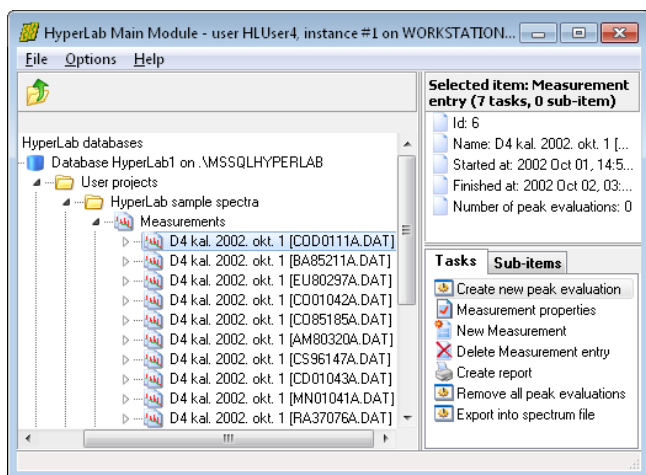
You should check the *Calibrations* tab now, where the source of FWHM and energy calibrations should be set to Spectrum files' own calibration values.

Click *Load files* button in order to initiate the spectrum loading.

All selected spectrum files will be loaded now, and the importer will provide basic information on the loading process.

Click *Close* to finish loading.





The database browser now displays the imported spectra. Now we will complete their missing *sample* settings.

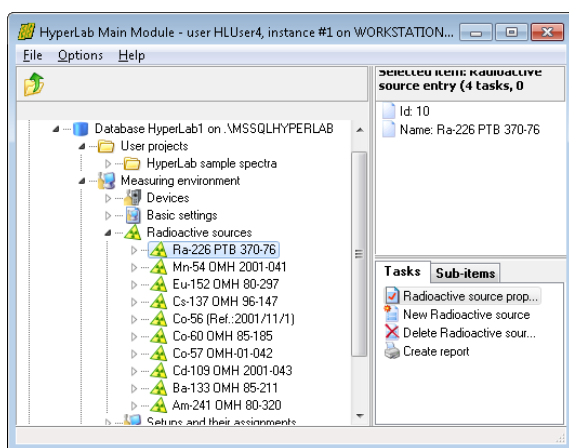
The sample is important presently only for calibration measurements, serving as input for later nonlinearity, efficiency and resolution analyses. These analyses will identify gamma lines by using isotope information, which is in turn supplied by the user, during the sample definition.

Radioactive source details

HyperLab's sample spectra are taken with the following radioactive sources:

Spectrum file	Source name	Activity	Act. unc.	Ref. date
AM80320A.DAT	Am-241 OMH 80-320	221.50 kBq	1.0 %	1 Oct 1980
BA85211A.DAT	Ba-133 OMH 85-211	456.40 kBq	1.5 %	1 Oct 1985
CD01043A.DAT	Cd-109 OMH 2001-043	100.44 kBq	0.5 %	1 May 2001
CO01042A.DAT	Co-57 OMH-01-042	32.63 kBq	0.5 %	1 May 2001
CO85185A.DAT	Co-60 OMH 85-185	434.60 kBq	0.7 %	1 Oct 1985, 12:00
COD0111A.DAT	Co-56 (Ref.:2001/11/1)	-	-	-
CS96147A.DAT	Cs-137 OMH 96-147	20.75 kBq	1.5 %	1 Dec 1996, 12:00
EU80297A.DAT	Eu-152 OMH 80-297	250.30 kBq	2.0 %	1 Dec 1980
MN01041A.DAT	Mn-54 OMH 2001-041	18.98 kBq	0.5 %	1 May 2001
RA37076A.DAT	Ra-226 PTB 370-76	112.00 kBq	0.667 %	1 Jan 1978

The corresponding radioactive sources must be created and assigned to the proper imported measurement. When no activity data is indicated, no absolute activity value is known. However, as only detector efficiency analysis uses intensity values of radiations, this may be disadvantageous only in that case.



To define a source, click the measurement and select its "Measurement properties" task. The measurement's property editor window appears now.

Please check if its *Source* field is set. If there is no reference to an existing source, or the *Measurement object type* field does not set to Source, then changes have to be made.

Set the *Measurement object type* field to *Radioactive source*, and check in the list of *Source* field's combo if the searched source is already defined. If it is already in the list, then select it, and click *OK* to finish editing of measurement entry.

If the source list does not contain the searched source, click the *Create new source entry* button beside the combo box. A source record editor page appears now. For further details on source entry editing, see section “Source properties editor window”.

The screenshot shows the 'Measurement properties' window with the following details:

- MEASUREMENT ID 1**
- MEAS. METHOD:** Decay-gamma measurement
- MEAS. SETUP:** D4 Setup 70keV - 3.3MeV, d=25cm
- PROJECT:** HyperLab sample spectra
- NAME:** D4 kal. 2002. okt. 1 [AM80320A.DAT]
- MEASURED BY:** Database administrator
- MEAS. OBJ. TYPE:** Radioactive source
- SOURCE:** Am-241 OMH 80-320
- STARTDATE:** 2002 Oct 10, 12:24:00, 001 msec
- ENDDATE:** 2002 Oct 10, 12:34:00, 000 msec
- EXPORT FILE NAME:** AM80320A

Note: Alternatively, instead of batch file importing, we could have loaded the spectra one by one, while supplying the sample information under the *Sample* tab for each spectrum file.

When all source data is properly set for each sample measurement, the loading of sample spectrum set is finished.

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