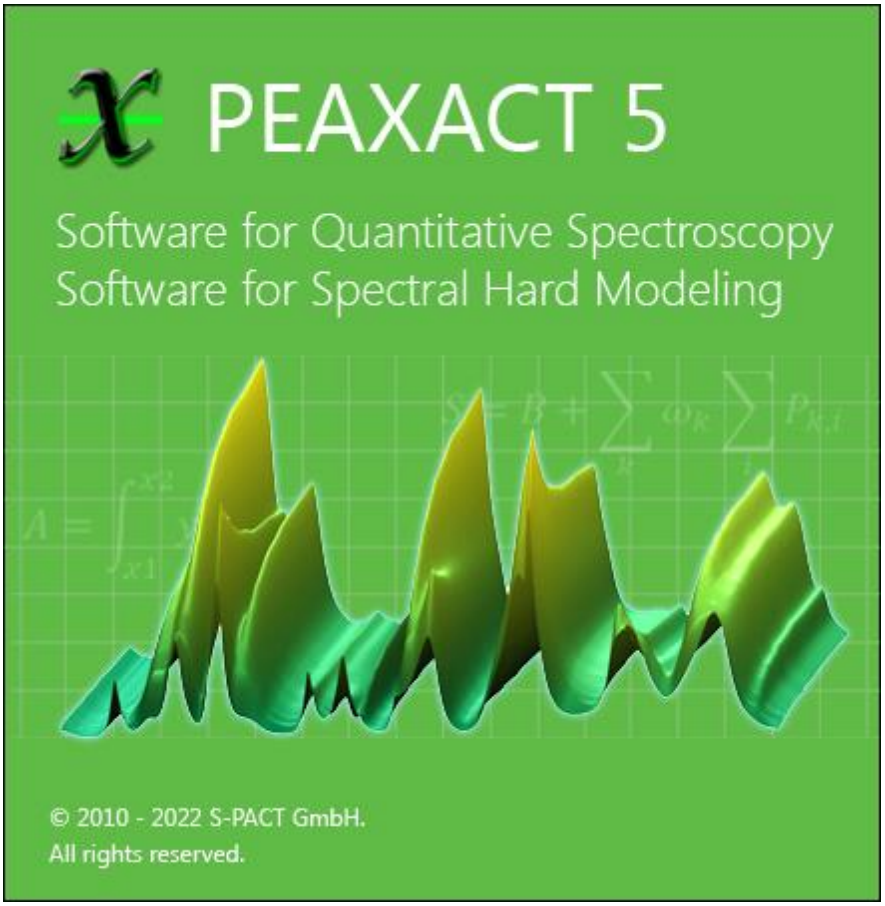
PEAXACT
User Manual

Version 5.9
2023-12-10



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1 QUICK START

1.1 What is PEAXACT?

PEAXACT is a comprehensive Windows application for the quantitative analysis of spectroscopic data using several state-of-the-art and innovative chemometric analysis methods. PEAXACT contains interactive tools for data visualization, exploration, modeling, classification, and calibration to identify and predict features from unknown samples. It offers quick-and-easy access to established methods like Peak Integration or Partial-Least-Squares and is the only software product that provides innovative ***Spectral Hard Modeling*** methods.

Separation to Related Software Products

PEAXACT is a Windows desktop application for interactive use. It is complemented by two related products, PEAXACT ProcessLink and PEAXACT AppServer, for the automated use in process analytics and reaction monitoring.

PEAXACT is optimized for spectroscopic data, e.g., IR, Raman, UV-Vis, and NMR spectra, but can be used for all kinds of peak-shaped signals in general. PEAXACT strongly focuses on quantitative data evaluation, i.e., determination of numerical properties from measured samples, though it also provides classification methods, i.e., determination of categorical properties.

PEAXACT does not ship with a spectral database for the identification of unknown substances from measured spectra. However, users can create their own database and train a Classification Model to achieve this functionality.

PEAXACT does not replace operating software for spectrometers. PEAXACT rather operates on data measured and saved with such software; it supports various third-party file formats.

PEAXACT is equipped with several data analysis methods. Some of these methods may also be distributed with other software. However, unique hard modeling methods like Indirect Hard Modeling (IHM) and Hard Modeling Factor Analysis (HMFA) are available in PEAXACT only.

1.2 Getting Help

User Manual

This user manual documents a certain version of PEAXACT. You can find the version number and release date on the title page.

We are continuously working on improving the manual. The latest document version is distributed as PDF file with each PEAXACT software update. The file is in subdirectory `Help` of the PEAXACT installation directory.

Technical Support

S-PACT Technical Support can be contacted in different ways:

- E-mail to support@s-pact.com
- Web form at www.s-pact.com/support
- From the PEAXACT main window (see Request Support)

> Note: A subscription of S-PACT Software Maintenance Service (SMS) is required to be eligible for technical support. The first year of SMS is included with new PEAXACT product licenses.

Blog

The PEAXACT Blog was launched as a free source of information complementary to the user manual. It contains tutorials and tips & tricks. See: blog.peaxact.com

1.3 Installation & License Activation

1.3.1 Requirements

- 64-bit version of Microsoft Windows 7 SP1 or Windows 10
- Any Intel or AMD x64 processor (four logical cores and AVX2 instruction set recommended)
- 5 GB of disk space (10 GB recommended)
- 4 GB RAM (8 GB recommended)
- No specific graphics card is required. Hardware accelerated graphics card supporting OpenGL 3.3 with 1GB GPU memory is recommended.

1.3.2 Licensing

PEAXACT software is furnished under a license agreement. The software may be used only under the terms of the license agreement.

License conditions vary with respect to license type, license option, and license modules. This section only gives a short overview of the different license options. For the full and legally valid conditions please refer to the license agreement document.

> Note: Depending on the modules of your license, you may not be able to access all PEAXACT features.

License Options

`Individual`	PEAXACT can be installed and operated by a single designated named user on up to 2 designated computers.

`Group`	PEAXACT can be installed on a specified number of computers and can be operated by an unlimited group of users (one user per computer at a time).
`Network`	PEAXACT can be installed on any number of computers in a network and can be operated by a specified number of users simultaneously. Licenses are shared among all network users. This option requires the PEAXACT License Server.

1.3.3 Installation

Step 1: Before You Install

- Make sure your computer fulfills the system requirements.
- When upgrading an existing installation, visit www.peaxact.com/whatsnew and read the upgrade notes and compatibility considerations.
- Make sure you have administrator privileges to perform the installation.
- Make sure your license is valid for the major version number. If you do not have a license yet you can get a free trial license or purchase a license after installation.

Step 2: Install PEAXACT

- Download the PEAXACT Installer from www.peaxact.com/download

> Note: The installer's file name is `PeaxactInstaller_<major>.<minor>_win64.exe`. Different major versions can be installed side-by-side, e.g., versions 5 and 4. The installer upgrades earlier installations of the same major version.

Online Installation

- Run the PEAXACT Installer and follow the setup instructions. Additional runtime packages are downloaded and installed automatically if detected missing.

Offline Installation

- If you are planning to install PEAXACT on a computer without internet access, you must download additional runtime packages in advance from www.peaxact.com/runtime
- Save all installer files to a folder on a portable drive. Do not rename files.
- At the offline computer, run the PEAXACT Installer and follow the setup instructions. Runtime packages are installed automatically if detected missing.

Step 3: After Installation

- After a new product installation continue with License Activation.
- After upgrading an existing installation check the upgrade notes at www.peaxact.com/whatsnew for further upgrade steps.

1.3.4 License Activation

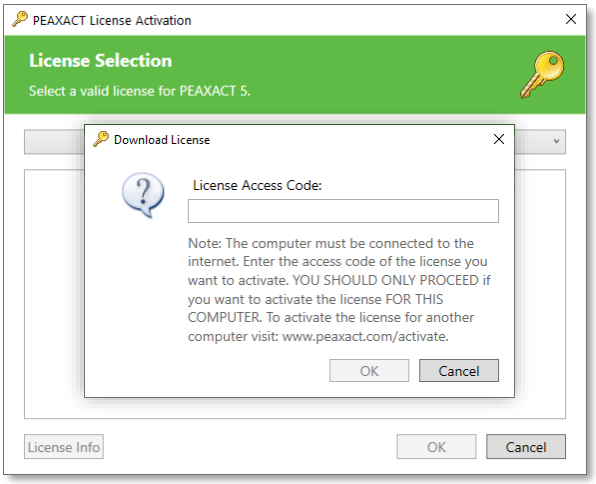
> Note: A **license access code** may be required for activation. Codes are provided to end-users or designated license administrators after a license purchase or trial request.
> Note: If you perform the activation with administrator privileges, licenses will be activated **per-machine**, i.e., for all Windows users. Otherwise, licenses will be activated **per-user**, i.e., for the logged-on user. Per-machine takes precedence over per-user.

Select **PEAXACT 5 > Activate PEAXACT** from the Windows start menu to open the License Activation Dialog. Then select the **PEAXACT Desktop App** product.

Online Activation

To activate PEAXACT over the internet:

- Select **Download License...** from the drop-down list.

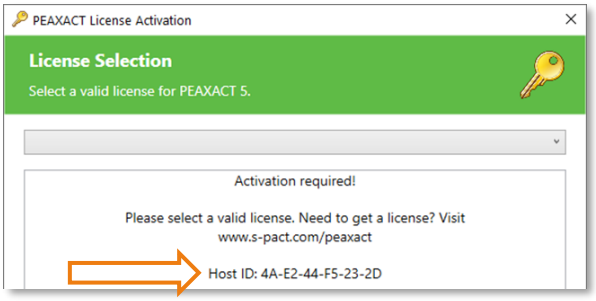


- Enter your license access code and click **OK**. Then close the dialog.

Offline Activation

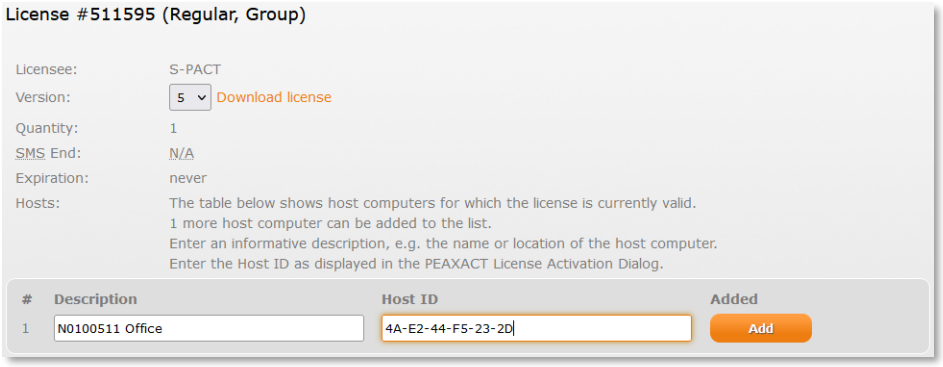
To activate PEAXACT on a computer without internet you must download the license using another device.

- Make a note of the **Host ID** displayed in the License Activation Dialog.



- On a device with internet, visit www.peaxact.com/activate.

- Sign in to the License Center with your license access code.

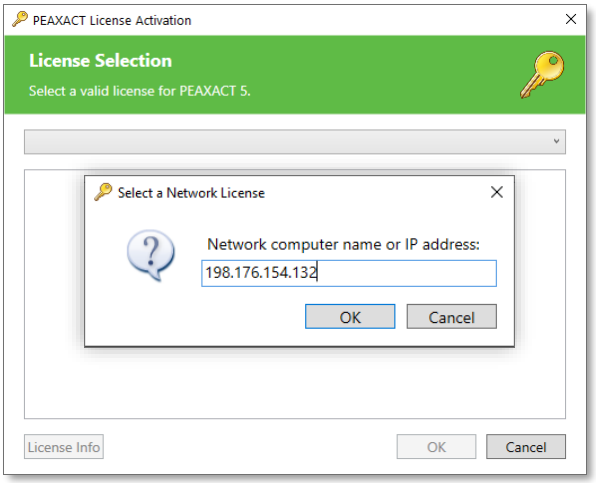


- Enter a description (e.g., the computer name) and the **Host ID**, then click **Add**.
- Click **Download license** and save the license file to a portable device.
- In the License Activation Dialog, select **Import License…** and load the license file. Then close the dialog.

Network Activation

To activate PEAXACT over the local network, the PEAXACT License Server must be running on a server computer.

- Select **Check-out from License Server…** (if available) from the drop-down list.



- Enter the computer name or IP address of the server computer and click **OK**.
- Select a license from the list and click **OK**. Then close the dialog.

1.4 Starting the PEAXACT Program

There are several ways to start the PEAXACT program on a Microsoft Windows platform:

- Click the Windows start menu and select **Programs** > **PEAXACT 5** > **PEAXACT 5**.
- Double-click the **PEAXACT 5 icon** on the Windows desktop.

- Open a command window, `cd` to the PEAXACT installation folder and type `Peaxact` at the command prompt.

After starting PEAXACT, a welcome screen opens while the program is loading.

> Note: Starting PEAXACT may need several seconds (up to a minute) for loading the MATLAB Runtime.

If you start PEAXACT without a valid license you will be prompted to activate a license.

If you have problems starting PEAXACT, see the Troubleshooting information.

Startup Options

PEAXACT can be started from the command line with additional parameters. Some command line options depend on the license. Type `PEAXACT -help` to see all available options for your license.

Parameters in square brackets are optional. Angle brackets represent placeholders which must be replaced by specific values. The vertical bar `(|)` separates alternative arguments.

```
PEAXACT
PEAXACT -help | -manual
PEAXACT [-debug]
        [-logfile <file>]
        [-openglfix]
        [-predict]
        [-restore | -session <file>]
        [<file1> [<file2> [...]]]
```

`-help`	Displays help for command line usage.
`-manual`	Opens the user manual.
`-debug`	Enables verbose log messages.
`-logfile <file>`	Specifies the log file. `<file>`: The path of a log file. The path must be put in double quotes if it contains spaces, e.g., `"c:\some folder\peaxact 5.log"`
`-openglfix`	Fixes graphics problems with some video cards.
`-predict`	Runs a prediction from the command line. Requires a calibrated model and sample files to be loaded. The option must be combined with options `-restore` or `-session <file>` and/or `<file*>` to load models and samples for the analysis. Running predictions from the command line has advantages over the graphical user interface. Learn more in section Prediction.

`-restore`	Reloads the most recently saved session.
`-session <file>`	Loads a session file. `<file>`: The path of a session file. The path must be put in double quotes if it contains spaces, e.g., `"c:\some folder\my session.pxs"`
`<file*>`	Loads additional files. These can be model files, sample files, or data table files. Multiple file paths must be separated by spaces. A path must be put in double quotes if it contains spaces, e.g., `"c:\some folder\file A.pxm"`

2 INPUT AND OUTPUT FILES

This section explains file types used by PEAXACT.

2.1 Model File

The central element of PEAXACT is a model which can be saved to and loaded from a file. A model file stores one model including all its sub-models and settings.

PEAXACT is backward compatible. It will read model files saved by all previous versions.

Supported File Formats for Reading

`*.fpm`	PEAXACT 2.x model file.

Supported File Formats for Reading and Writing

`*.pxm`	PEAXACT model file since version 3.

2.2 Sample File

A sample file contains one or more samples, each of which consists of x-data (wavenumbers, frequencies …) and y-data (intensities). PEAXACT supports various file formats including some 3D formats (files containing multiple samples), and 4D formats (files containing multiple frames of multiple samples).

Sample URI

PEAXACT uses a uniform resource identifier (URI) to unambiguously identify a specific sample in a 2D, 3D, or 4D sample file. The URI is composed of the file path followed by the number sign `#` and a sample ID (e.g., `c:\data\mixture.txt#3`). URIs without number sign and ID refer to all samples in the file. For most 2D sample files (single sample) and 3D sample files (multiple samples), the ID simply is the sample number within the file (e.g., `#3`). For 4D sample files (multiple frames), the ID is a combination of the frame number followed by the sample number within the frame (e.g., `#10-3`). Other format specific IDs are described below.

Supported File Formats for Reading

`*.0`	Bruker OPUS files. The sample ID is the OPUS block name followed by the sample number within the block (e.g., `#AB-3`).
`*.1d`	Magritek 1D files.

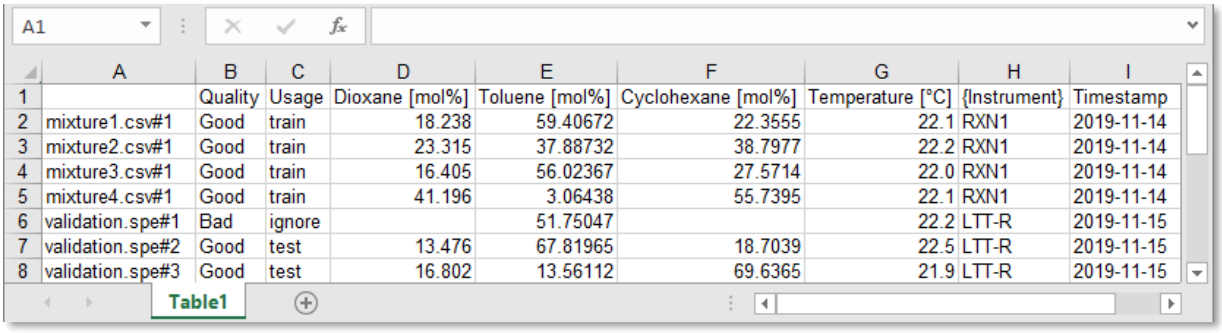
`*.cdf`	Agilent netCDF chromatogram files.
`*.csv *.tsv *.dpt *.txt`	Text files (delimiter separated values). Text files must contain tabularly structured data. The first table column is interpreted as x-data while following columns are interpreted as y-data. Table headers are ignored. The decimal separator should be a point. A decimal comma is also acceptable except when the delimiter character is a comma.
`*.dx *.jdx *.jcm`	JCAMP-DX files.
`*.mat`	Matlab MAT files. Files must contain one numeric matrix variable. The variable's name can be arbitrary. The first matrix column is interpreted as x-data while following columns are interpreted as y-data.
`*.sp`	Perkin Elmer files.
`*.spa *.spg *.srs`	Thermo Nicolet OMNIC files.
`*.spc`	Galactic SPC file.
`*.spe`	WinView files, WinSPEC files, LightField files.
`*.spv`	Spekwin32 files.
`*.tdms`	LabVIEW TDMS files. Files can contain any number of named groups, each of which can contain any number of named channels, each of which contains data points. Data are recognized when a group contains two channels with the same number of data points. The first of those channels is interpreted as x-data, the second one as y-data. Group names and channel names can be arbitrary. The sample ID is the group name (e.g., `#Spectrum`).
`*.wdf`	Renishaw WiRE files.

Supported File Formats for Writing

`*.csv`	Text files (delimiter separated values). The delimiter for writing text files is set by a user preference.
`*.mat`	Matlab MAT files.

2.3 Data Table File

A PEAXACT data table file is a spreadsheet file in which each row represents a sample and columns represent sample URIs and sample features. The concept of data tables is an easy way to manage data that belongs together. See also Data Management for further information.



	A	B	C	D	E	F	G	H	I
1		Quality	Usage	Dioxane [mol%]	Toluene [mol%]	Cyclohexane [mol%]	Temperature [°C]	{Instrument}	Timestamp
2	mixture1.csv#1	Good	train	18.238	59.40672	22.3555	22.1	RXN1	2019-11-14
3	mixture2.csv#1	Good	train	23.315	37.88732	38.7977	22.2	RXN1	2019-11-14
4	mixture3.csv#1	Good	train	16.405	56.02367	27.5714	22.0	RXN1	2019-11-14
5	mixture4.csv#1	Good	train	41.196	3.06438	55.7395	22.1	RXN1	2019-11-14
6	validation.spe#1	Bad	ignore		51.75047		22.2	LTT-R	2019-11-15
7	validation.spe#2	Good	test	13.476	67.81965	18.7039	22.5	LTT-R	2019-11-15
8	validation.spe#3	Good	test	16.802	13.56112	69.6365	21.9	LTT-R	2019-11-15

Supported File Formats for Reading and Writing

`*.xls`	Excel 97-2003-workbook.
`*.xlsx`	Excel workbook.
`*.csv`	Text files with tabular data separated by a delimiter character. Note that PEAXACT supports the `csv` file extension for both sample files and data table files. To avoid confusion, it is recommended to use Excel files for data tables if possible.

Table Layout

PEAXACT can read data table files of the following layouts:

A) Sample URIs only.	The table only consists of a single column which is a list of sample URIs. Loading the table loads all referenced sample files.
B) Sample features only.	The table does not contain sample URIs, but only consists of columns with numerical or categorical feature values. Such a table cannot be loaded directly but must be joined with previously loaded samples. See Join Table.
C) URIs and Features.	The table is a combination of A) and B) containing both sample URIs and feature values. Loading the table loads all referenced sample files and associated features.

Table Format

PEAXACT can read data table files if the following formatting rules apply:

- Layouts A, C: First table column contains sample URIs (absolute or relative path).
- Layouts B, C: First table row contains feature names (except for first column).
- Rows without URI as well as columns without feature name are ignored.
- Feature names can be anything. When put in curly braces (e.g., `{Group}`) features are treated as categorical, otherwise as numerical.
- Values of numerical features must be numeric. Values of categorical features can be text or numbers, though numbers are treated as text.
- The following feature names are special and treated differently:
  - `Quality`: values can be `Good` or `Bad`
  - `Usage`: values can be `train`, `test`, or `ignore`
  - `Timestamp`: date and/or time as text or serial number
- Empty cells are interpreted as missing values.
- In case of duplicate URIs, feature values are merged (values from rows further down take precedence over values from rows further up).
- In case of duplicate feature names, only the first occurrence is considered.
- For Excel files, only the first worksheet is considered.

2.4 Session File

A session file is a snapshot of the PEAXACT workspace. You can save the current session and load it later to restore the workspace and continue working where you stopped before.

Supported File Formats for Reading

`*.mat`	PEAXACT 2.x Session file.

Supported File Formats for Reading and Writing

`*.pxs`	PEAXACT Session file since version 3.

Auto-Save

PEAXACT can automatically save session files on shutdown (see preferences). Those files are saved in `%LocalAppData%\S-PACT\PEAXACT 5\Sessions`

2.5 Session Profile File

A session profile contains session-related preferences. PEAXACT is shipped with pre-defined profiles for typical applications. Profiles can be added, removed, or modified with the Preferences Editor, and changes can be saved to or loaded from a profile file.

Supported File Formats for Reading and Writing

`*.profile`	PEAXACT session profile.

Profile Directory

When not specified otherwise, profiles are saved to and loaded from the default directory `%LocalAppData%\S-PACT\PEAXACT 5\Profiles`

2.6 License File

The license file contains PEAXACT licensing details. On startup, PEAXACT searches the Windows registry for a registered license file or displays the License Activation Dialog to load a new license.

Supported File Formats for Reading

`*.lic`	PEAXACT License file.

2.7 Report File

Report files are used to export graphical or tabular reports. Depending on the report, different file formats are available such as text, table, or image files.

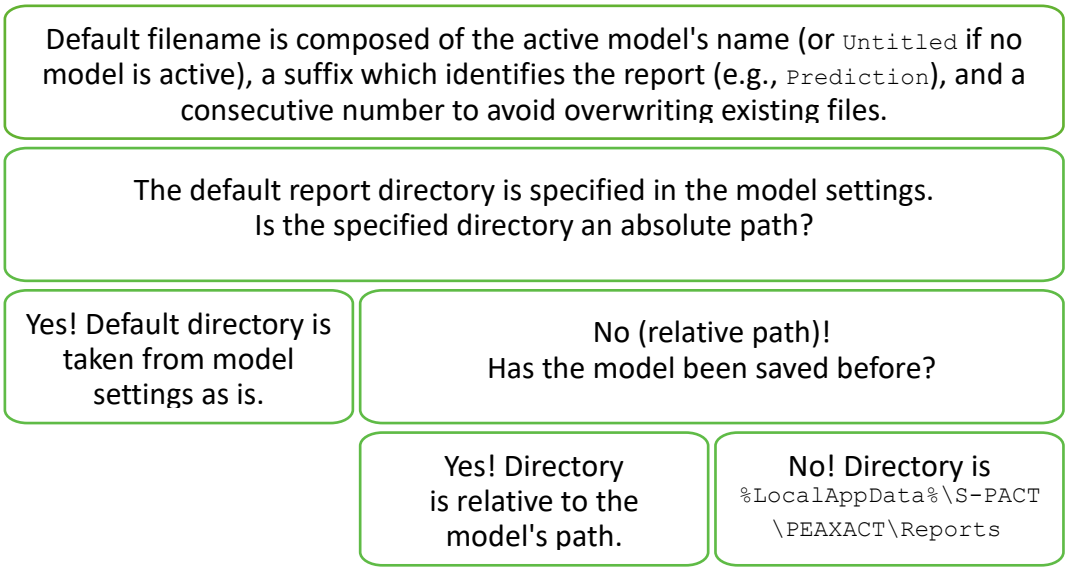
Supported File Formats for Writing

`.pdf`	Portable Document Format.
`.xls`	Microsoft Excel 97-2003 Workbook.
`.xlsx`	Microsoft Excel Workbook.
`.csv`	Comma separated values.
`.dpt`	Tab separated values.
`.txt`	Blank separated values.
`.jpg`	JPEG image file.
`.png`	PNG image file.
`.tiff`	TIFF image file.
`.bmp`	Bitmap image file.

`.eps`	Encapsulated PostScript image file.
`.fig`	Matlab figure file.

Default Directory and Filename

Writing reports typically involves a File Dialog which you can use to browse directories and choose a filename. A default filename is suggested according to the heuristic below. Default filenames are used automatically when PEAXACT is running in non-interactive mode.



2.8 Log File

PEAXACT writes messages, warnings, and errors to a log file. The log file path can be changed with the command line parameter `-logfile`. The verbosity of log messages can be increased using the command line parameter `-debug`.

Default File Path

`%LocalAppData%\S-PACT\PEAXACT 5\Peaxact.log`

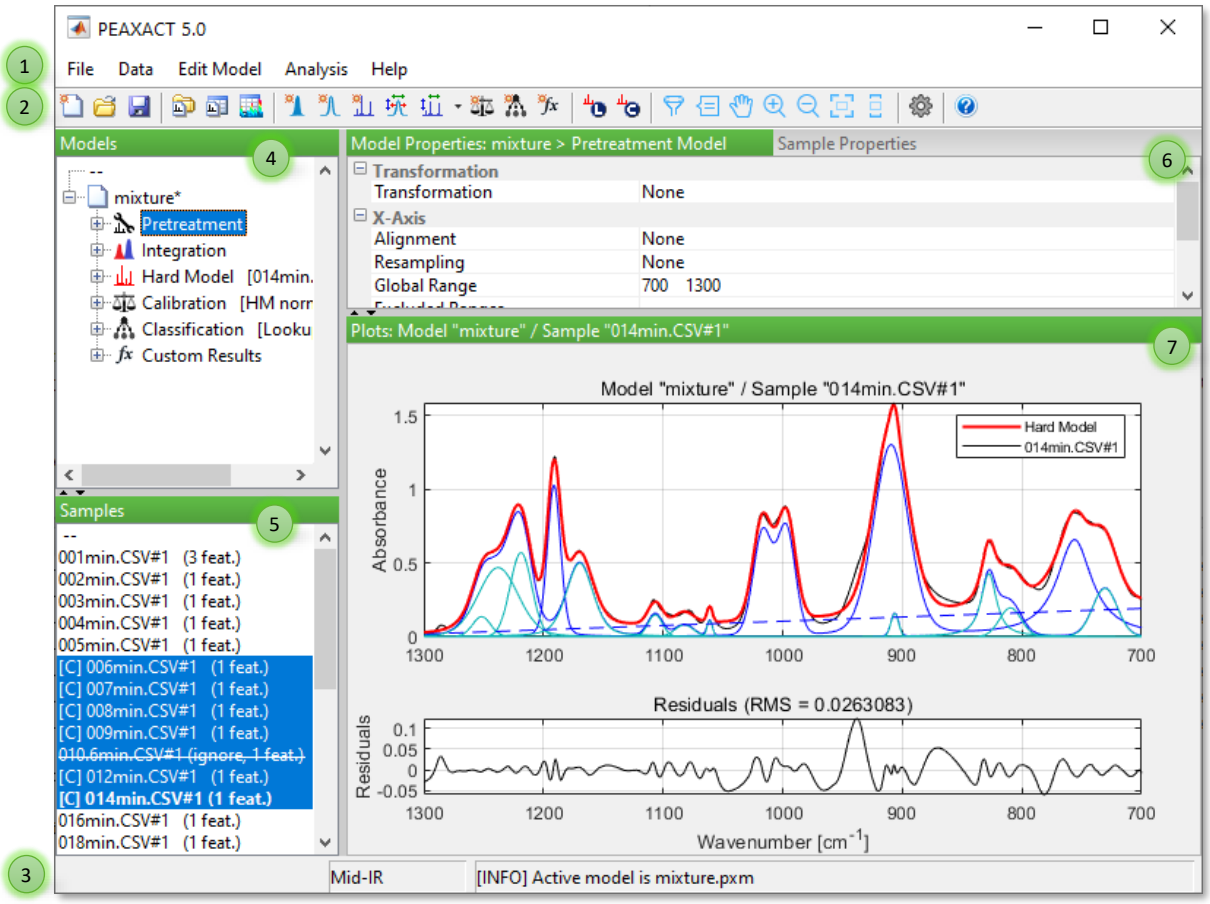
3 PEAXACT USER INTERFACE

The PEAXACT graphical user interface consists of multiple interactive windows. Features include:

- 2D and 3D data visualization
- Data pretreatments specifically suited for spectroscopic data
- Interactive data modeling, including ***Spectral Hard Modeling***.
- Qualitative and quantitative analyses, e.g.
  - Peak Picking
  - Integration
  - Principal Component Analysis (PCA)
  - Cluster Analysis
  - Rank Analysis based on Principal Components
  - Multivariate Curve Resolution (MCR-ALS)
  - Hard Modeling Factor Analysis (HMFA)
  - Peak Fitting / Peak Deconvolution / Indirect Hard Modeling (IHM)
  - Component Fitting
  - Univariate Regression and Prediction
  - Partial Least-Squares (PLS) Regression and Prediction
  - Identification with Lookup Tables
  - Identification with Discriminant Models
  - User-defined Custom Results
- Customizable reporting
- Exporting to several output formats

3.1 Main Window

When you start the PEAXACT program it displays the main window. The main window contains controls for managing, modifying, and displaying models and samples.



PEAXACT main window with models and samples

1) Menu bar
2) Toolbar
3) Status bar
4) Model Tree Panel
5) Samples Panel
6) Properties Panel
7) Plot Panel

The main window is structured into four panels. Drag the gray bar between two panels to resize them or hide/re-show panels by clicking the arrows on the resize bar.

3.1.1 Menu bar

Use the menu bar to access actions by category.

File	Model File Management, Preferences, Sessions
Data	Data Management, Data Inspector
Edit Model	Modeling Tools
Analysis	Analysis & Reporting
Help	Documentation, Support, Licensing, Web Resources...

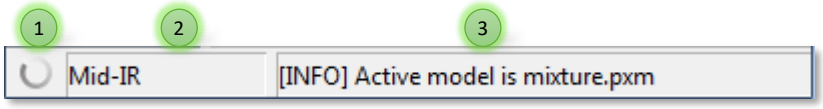
3.1.2 Toolbar

Use the toolbar to quickly access frequently used actions.

	New Model, Open Model, Save Model
	Load Samples, Load Data Tables
	Data Inspector
	Add Integration Model Peak Add & Auto-fit Hard Model Peaks Import Hard Model Components Adjust Hard Model Peaks Adjust Hard Model Components New Calibration Model New Classification Model Add Custom Result
	Linear Component Fit preview Component Fit preview according to Hard Model settings
	Data Filter Tool, Data Cursor Tool, Pan Tool, Zoom In Tool, Zoom Out Tool, Full Zoom, Full Y-zoom
	Preferences Editor
	User Manual

3.1.3 Status bar

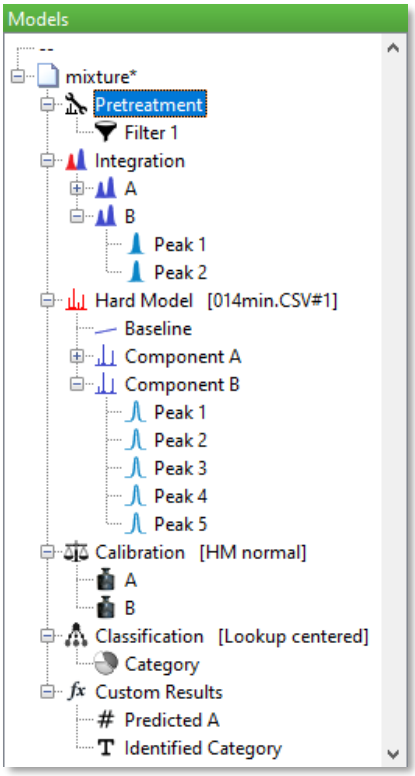
Use the status bar to obtain status information.



1) Busy Indicator: Indicates whether PEAXACT is currently busy and cannot respond to mouse-clicks or pressed keys.
2) Current Profile: Displays the currently active session profile. Left-click to open the Preferences Editor.
3) Status Message: Displays the status of the last action carried out. Left-click to open the message window, where all recent status messages are displayed.

3.1.4 Model Tree Panel

The Model Tree Panel displays opened model files, each represented by a tree structure. Use the tree to access certain model elements.



--	Empty item. Select this if no model should be active.

Model Name	Each top-level tree item represents a model file. The displayed model name corresponds to the file name, marked with an asterisk (*) if the model has unsaved changes.
Pretreatment	Pretreatment Model: the sub-model with options for the manipulation of the sample signal. Pretreatments are applied prior to all other operations.
Name	Data Filter: a named x-region of the sample signal to be used for further operations (after pretreatments), mainly for PLS calibration.
Integration	Integration Model: the sub-model for the calculation of component areas from the sample signal by numerical integration.
Name	Integration Model Component: a named container for Integration Model Peaks, representing a chemical component. The component area is the sum of its peak areas.
Peak *N*	Integration Model Peak: defines x-limits and a baseline for the numerical integration of the sample signal.
Hard Model [*Sample*]	Hard Model: the sub-model for the calculation of component weights from the sample signal by fitting peak curves. The name of the sample to which the model was last fitted is displayed in brackets.
Baseline	Hard Model Baseline: a linear or quadratic curve which is fitted to the sample signal along with Hard Model Components.
Name	Hard Model Component: a named container for Hard Model Peaks, representing a chemical component. The component weight is a scaling factor for its peaks.
Peak *N*	Hard Model Peak: defines the position and shape parameters of a peak curve to be fitted to the sample signal.
Calibration [*Method*]	Calibration Model: the sub-model for the quantitative conversion of the sample signal to numerical features by means of univariate or multivariate regression. The calibration method is displayed in brackets.
Name	Calibration Model Component: a named component trained with reference samples to predict feature values from unknown samples.
Classification [*Method*]	Classification Model: the sub-model for the qualitative conversion of the sample signal to a categorical feature. The classification method is displayed in brackets.

Name	Classification Model Component: a named component trained with reference samples to identify feature classes from unknown samples.
Custom Results	Custom Results: the sub-model for user-defined results.
Name	Numerical Result: a named custom result returning a number.
Name	Categorical Result: a named custom result returning text.

Selecting and Activating Models

Use the mouse, e.g., to select an element from the tree. This activates the model to which the element belongs. Note that only one model can be active at a time. Many operations of PEAXACT implicitly operate on the active model.

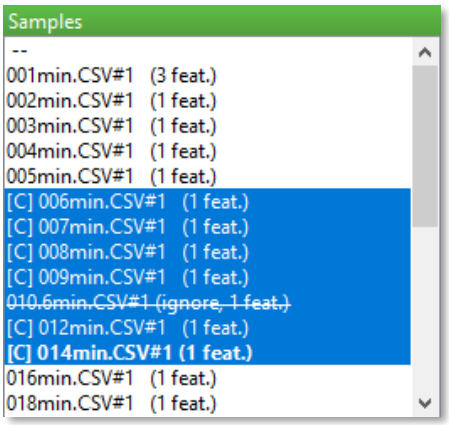
Selecting model elements affects other parts of the main window:

- Display of the element's parameters (see Properties Panel)
- Display and/or highlighting of the element's plot (see Plot Panel)
- Enabling of element-specific actions in the Menu bar and Toolbar

Sometimes it is favorable to not have any model active. Select the empty item (--) for this purpose.

3.1.5 Samples Panel

The Samples Panel shows a list of loaded samples. Use the panel to access certain samples.



--	Empty item. Select this if no sample should be active.

Sample Name	Each item represents a sample. The sample name is composed of the sample filename and ID (see Sample File). Additional information, if any, may be added to the name: The name is crossed out if the feature `Quality` is set to `Bad`. `test` or `ignore` indicate the value of feature `Usage`. The default value `train` is not shown. `t` indicates that a `Timestamp` is available. `#feat.` indicates the number of other available features. `[C]` indicates that a Component Fit exists.

Selecting and Activating Samples

Use the mouse, e.g., to select one or more samples from the list. Press `CTRL+A` to select all samples. The last selected sample becomes the active sample, noticeable by its name being displayed in bold letters. Many operations of PEAXACT – including all analyses – are applied to the selected samples; some operations implicitly operate on the active sample.

When activating a sample whose URI points to a missing file you are prompted to Update Missing Files.

Activating a sample affects other parts of the main window:

- Display of the sample's spectrum (see Plot Panel)
- Enabling of specific actions in the Menu bar and Toolbar

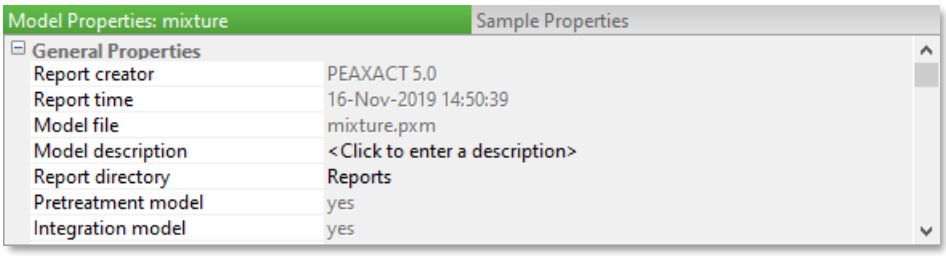
Sometimes it is favorable to not have any sample active. Select the empty item (--) for this purpose.

3.1.6 Properties Panel

The Properties Panel displays either Model Properties or Sample Properties. Switch between the two by clicking on the respective heading.

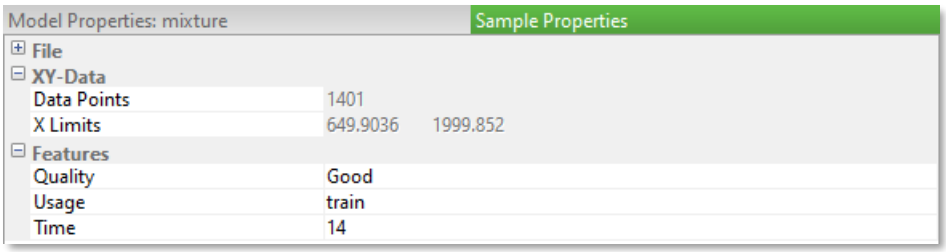
Model Properties

Use the Model Properties Panel to get and set properties of the model currently active in the Model Tree Panel. Visible properties depend on the selected model element. Some properties are read-only, others are editable.



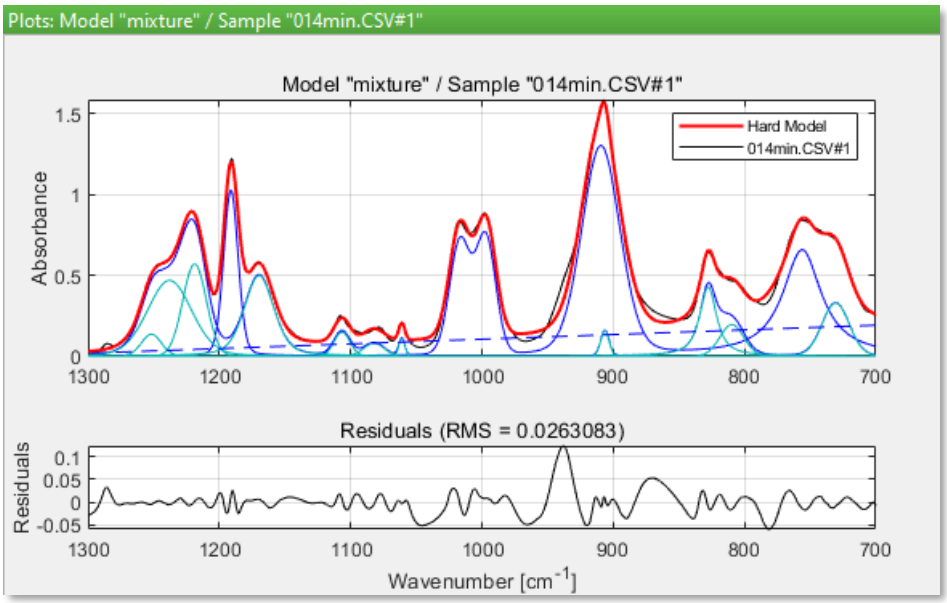
Sample Properties

Use the Sample Properties Panel to get and set properties of the sample currently active in the Samples Panel. Properties are grouped into categories. Categories **File** and **XY-Data** are read-only, category **Features** is editable.

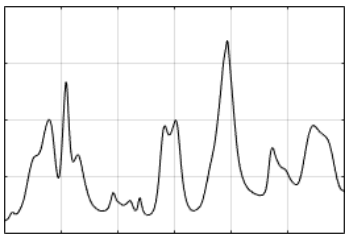


3.1.7 Plot Panel

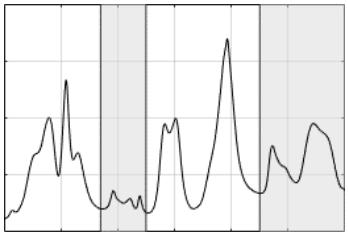
The Plot Panel contains a graphical display of the items selected in the Model Tree Panel and in the Samples Panel. Use the mouse, e.g., to interact with the plots to select and edit model elements.



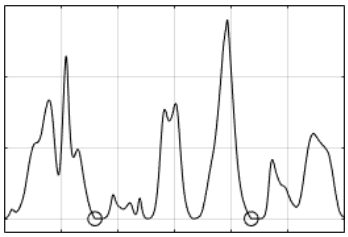
Available Graphs



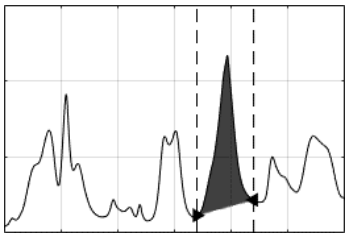
Sample Spectrum
Graph of the active sample's spectrum (black line). If a model is active in the Model Tree Panel, the sample is modified according to the active model's Pretreatment Model. The sample plot cannot be modified interactively. (Hint: Use the Data Inspector to plot multiple samples)



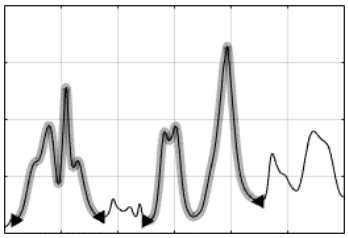
Pretreatment Model – Excluded Ranges
Graph of excluded ranges (transparent gray patches) of the active model's Pretreatment Model. Excluded ranges can be modified with the mouse (see preferences).



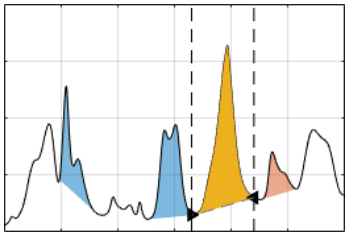
Pretreatment Model – Rubber Band Baseline Nodes
Graph of rubber band baseline nodes (black circles at y = 0) of the active model's Pretreatment Model. Baseline nodes can be modified with the mouse.



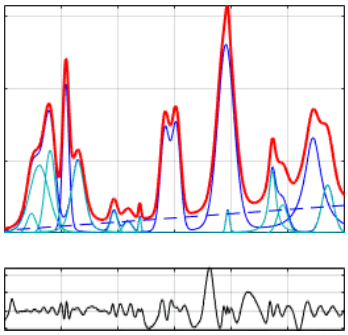
Pretreatment Model – Reference Peak for Normalization
Graph of the reference peak for normalization of the active model's Pretreatment Model. The reference peak can be modified with the mouse.



Data Filter
Graph of the currently selected Data Filter of the active model's Pretreatment Model. The Data Filter can be modified with the mouse.



Integration Model
Graph of peaks of the active model's Integration Model (colored areas). Integration Model Peaks can be modified with the mouse.



Hard Model and Residuals
Graph of baseline (dashed blue line), components (solid blue lines), and peaks (cyan lines) of the active model's Hard Model (red line). Baseline and peak plots can be modified with the mouse (when not in component fit preview mode).

If a sample is active in the Samples Panel, the sample spectrum is plotted too, and the differences (residuals) between Hard Model (red line) and sample (black line) are shown in a second graph.

Interactive Modeling

Most model-related graphs can be modified interactively with the mouse. Available actions differ from graph to graph but typically include:

- left-clicking a graph to select the corresponding element in the Model Tree Panel
- dragging a graph while the left mouse-button is pressed to change the graph's position or shape
- right-clicking a graph to open the corresponding context-menu
- hitting the DEL-key to delete the selected element from the model
- hitting the F2 key to rename the selected model element

Detailed descriptions can be found in section Modeling.

3.2 Working in Sessions

A PEAXACT session contains models and samples, and represents an isolated environment where analyses execute. By default, PEAXACT starts with an empty session where you can create models and load samples. You can also create new sessions, save the current session to a session file or load a saved session file to continue working where you left before. Each session has associated settings (see Session Profile) that can be adjusted to the kind of data you want to work with, e.g., Raman spectra or NMR spectra.

3.2.1 New Session

Menu bar:	File > New Session > (Profile)

When starting a new session, you must pick a session profile to work with. Starting a new session clears the current workspace and resets the main window to its initial state: all windows except the main window are closed, all model files are closed, and all sample files are unloaded.

You will be asked to save the current session first.

3.2.2 Open Session

Menu bar:	File > Open Session > Load Session File…
Menu bar:	File > Open Session > …

You can choose between loading a session from file (by using the File Dialog) and reloading a recently opened session.

When opening a session file, the current session is closed, and the workspace of the opened session is restored.

Drag and Drop

A fast way to open a session file is by using drag & drop. Drag a single session file from the Windows Explorer (e.g.) and drop it into the Model Tree Panel or the Samples Panel. Note: if you drag & drop multiple files, PEAXACT ignores any session files among them and tries to open model files or sample files instead.

Command Line Alternatives

```
peaxact -session <file>
peaxact -restore
```

When starting PEAXACT from the command line, you can pass additional parameters to either open a certain session file or to restore the most recently saved session.

What is Restored from Session Files?

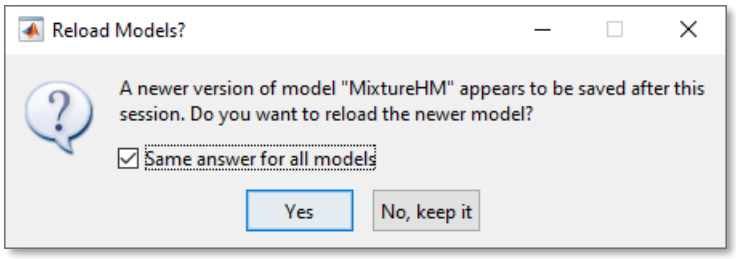
- Models are restored exactly to the state when the session was saved (see below).
- Samples are restored exactly to the state when the session was saved, including filenames. When you move or rename these files on your hard disk, filenames stored in the session still point to the old location and need to be updated after the session is restored (see below).
- Component Fits
- Selected and active elements of the Model Tree Panel and Samples Panel are restored. Therefore, the Properties Panel and Plot Panel also are restored to their previous state.
- Session settings

Caution with Models Restored from Sessions!

A model restored from a session file must be treated with care, especially if

- multiple sessions exist containing the model at different building stages
- the model was modified and saved to file after the session was saved

In these cases, it is possible to restore a model from a session file which in the meantime has been replaced by a newer version. You can choose whether to reload the newer model or continue working with the one contained in the session file.



Update Missing Sample Files

Samples stored in a session file contain references (URIs) to files from the moment the session was saved. When you move or rename these files on your hard disk, filenames stored in the session still point to the old locations. After reloading a session, you may have to update these file references. PEAXACT informs you to update missing files when it tries to load data from a missing file.

3.2.3 Save Session

Menu bar:	File > Save Session As...

Use the File Dialog to browse directories and select a filename for the session to be saved.

When saving a session file, the current workspace is written to the hard disk.

Auto-Saving

The current session can be saved automatically to a special directory on PEAXACT shutdown (see preferences).

What is Stored in Session Files?

- Models. Note that unsaved model changes are not saved to model files. Therefore, these models will still be marked unsaved when the session is re-opened later.
- Samples
- Component Fits
- Selected and active elements of the Model Tree Panel and Samples Panel
- Session settings

3.3 Model Management

3.3.1 About Models

What are Models?

A model is a set of parameters used by PEAXACT algorithms to solve analysis tasks, e.g., predicting concentrations from measured spectra. Models are structured into sub-models for specific sub-tasks:

- Pretreatment Model: parameters for data manipulation.
- Integration Model: parameters for peak integration.
- Hard Model: parameters for peak fitting and component fitting.
- Calibration Model: parameters for quantitative analyses.
- Classification Model: parameters for qualitative analyses.
- Custom Model: user-defined expressions to calculate custom results.

Modeling and Analysis

The lifetime of a model passes at least two stages:

- First, an analysis method must be chosen, and appropriate model parameters must be set. This process is called modeling. The amount of information that must be provided during modeling depends on the analysis method. For instance, calibration methods require a Calibration Model; hard modeling methods require a Hard Model.
- After the model has been created, it can be utilized for analyses.

Getting Access to Model Parameters

The Model Tree Panel is a graphical control designed for browsing the model's structure. It quickly gives an overview of all the sub-models and their content. The model tree can be used to select any element of the model and then get displayed additional information about that element in the Properties Panel.

For most model elements, the Properties Panel gives access to model parameters and their values. When clicking the model item in the Model Tree, the Properties Panel displays a summary of the most important parameters in a tabular report.

Model File

The model file is a physical file on the hard disk which is written by PEAXACT and stores all model parameters.

Exporting Reports

Menu bar:	File > Export > ...

Model reports are tabular or graphical representations of model parameters. Model reports can be re-created at any time because the necessary information is persistently stored within the model file. PEAXACT can export reports to different output formats such as XLS or PDF.

The following model reports are available:

Model Summary	A tabular summary of model parameters. This report is also displayed in the Properties Panel after selecting the top-level model item in the Model Tree Panel.
Model Details	A full tabular report of all model parameters for documentation purposes.
Hard Model XY Data	A table containing y-values of the Hard Model calculated at x-values of the active sample. The data can be used to reproduce plots of the Hard Model like those in the Plot Panel.
Calibration Data Table	A PEAXACT data table containing sample URIs and feature values used to create the Calibration Model.
Classification Data Table	A PEAXACT data table containing sample URIs and feature values used to create the Classification Model.
Plot	This report exports the current content of the Plot Panel to an image file.

3.3.2 New Model

Toolbar:	
Menu bar:	File > New Model
Hot key:	CTRL + N
Context menu:	Model Tree Panel > New Model

Adds a new model to the Model Tree Panel.

Model Name

The new model's name is "Untitled" by default. If an opened model already has this name, a consecutive number is added.

A model is always named after its filename. To rename a model in PEAXACT, save it under a new filename. To rename a model outside PEAXACT, simply rename the file. Caution: Do not change the file extension!

Initial Settings

Each time a new model is created, initial settings are copied from the then-active session profile. You can later modify model settings of each model individually in the Model Properties Panel.

3.3.3 Open Model

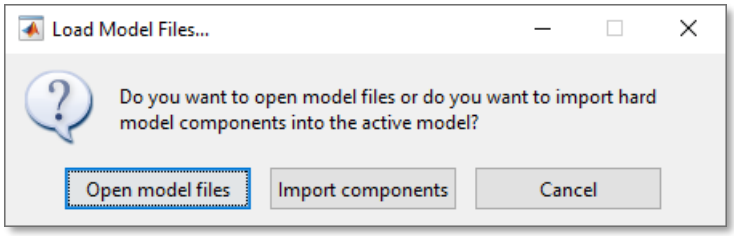
Toolbar:	
Menu bar:	File > Open Model...
Hot key:	CTRL + O
Context menu:	Model Tree Panel > Open Model...
Drag & drop:	from Explorer to Model Tree Panel

Opens a previously saved model file. A File Dialog can be used to browse directories and select one or more model files to be opened. Choose a file filter from the drop-down list to localize certain model files. Opened models are added to the Model Tree Panel.

Drag and Drop

A fast way to open model files is by using drag & drop. Drag any files from the Windows Explorer (e.g.) and drop them into the Model Tree Panel. Hint: If your directory contains many different files, you can simply select all files and drop them to the Model Tree Panel. PEAXACT automatically filters out model files. You may also drag & drop directories to load all model files from the directory.

If any model is active while dropping files to the Model Tree Panel, you will be asked whether to open these files or to import components into the active model.



Reload Open Model

If you open a model file that is already opened, you will be asked whether to reload the model or discard all unsaved changes (if any).

3.3.4 Close Model

Menu bar:	File > Close Model
Hot key:	CTRL + W
Context menu:	Model Tree > Model Item > Close

Closes the active model file. The model is removed from the Model Tree Panel and the next available model becomes active.

Unsaved Changes

If the active model contains unsaved changes, you will be asked to save the model first. Otherwise, the model file is closed directly.

3.3.5 Close All

Menu bar:	File > Close All

Closes all model files. This is a fast way to clear the Model Tree Panel. If any model has unsaved changes, you will be asked whether to save them or discard changes.

Closing Models on Shutdown

All models will be closed when closing the PEAXACT main window. Respectively, you get the chance to save unsaved changes.

3.3.6 Save Model

Toolbar:	
Menu bar:	File > Save Model
Hot key:	CTRL + S
Context menu:	Model Tree > Model Item > Save

Saves the active model to its file. If the model has never been saved before PEAXACT falls back to Save As.

3.3.7 Save Model As

Menu bar:	File > Save Model As...
Context menu:	Model Tree > Model Item > Save As...

Saves the active model to a new file. A File Dialog can be used to browse directories and select or enter a filename for the model to be saved.

Overwriting Existing Files

As a precaution, you cannot save a model to a file of another model that is currently opened in PEAXACT. You must close the other model before overwriting its file.

3.3.8 Duplicate Model

Menu bar:	File > Duplicate Model
Context menu:	Model Tree > Model Item > Duplicate

Creates an exact copy of the active model. The new model is added to the Model Tree Panel. The duplicate gets the name of the source model plus a consecutive number.

Using Duplicates

Using duplicates is useful if you already have a populated model and want to compare the effects of different model settings without changing the original model.

3.4 Data Management

3.4.1 About Samples

What are Samples?

In PEAXACT, the term *Sample* refers to the digital representation of a physical sample. Each digital sample at least consists of a spectrum (the sample's xy-data) and may have other features associated with it.

The Sample URI

Samples are stored in sample files. PEAXACT works with references to sample files, so called *uniform resource identifiers (URI)*. The reference is composed of a filename and – because the file may contain more than one sample – a sample ID. Each URI unambiguously identifies a specific sample. Learn more about URIs in section Sample File.

Example URI:

```
C:\Program Files\S-PACT\PEAXACT 5\Data\NIR - Gasoline\References\ NIR.mat#15
```

Sample Name

The *sample name* is a shortened URI, namely the sample file name and the sample ID. Sample names are often used in PEAXACT, e.g., in report dialogs, in result files, or as display names in the Samples Panel.

Example Name:

```
NIR.mat#15
```

Features

The term sample *feature* refers to any kind of information that is associated with a sample. Each feature has a name and a numerical or categorical (text) value. Respectively, features are called

either *numerical features* or *categorical features*. PEAXACT uses the feature name to distinguish between numerical and categorical features. There are also some reserved names for special features. The following table describes all types of features:

`Numerical`	A feature is considered numerical if its name is neither put in curly braces nor is a special name (see below). Example names for numerical features: `Cyclohexane [mol%]`, `Pressure [bar]`, `Temperature [°C]`, `Octance Number`, `Salinity`. Although not required, it is recommended to include the unit of measurement in the name. The value of numerical features must be numbers.
`Categorical`	A feature is considered categorical if its name is put in curly braces. Example names for categorical features: `{Replication Group}`, `{Batch}`, `{Temperature Level}`, `{Operator Name}`, `{Instrument ID}`. The value of categorical features must be text or numbers, though numbers are treated as text.
`Quality`	A special feature name to label the quality of a sample. You can choose from a predefined set of values: `Good`: The sample is considered for all modeling operations and analyses. This is the default value. `Bad`: The sample is excluded from all modeling operations and all analyses. Assign this value, e.g., if the sample spectrum is an outlier or too noisy.
`Usage`	A special feature name to specify the usage of a sample for calibration or classification. You can choose from a predefined set of values: `Train`: The sample is used for training of the calibration/classification model. This is the default value. `Test`: The sample is used for validation. `Ignore`: The sample is not used for neither training not testing.
`Timestamp`	A special feature name to specify the acquisition date and/or time of the sample spectrum. The value must be either a date in the format `YYYY-MM-DD`, a time in the format `hh:mm:ss`, or a combination of both `YYYY-MM-DD hh:mm:ss`.

Sample features are used for many purposes:

- coloring and arranging 2D and 3D plots in the Data Inspector
- sorting samples in the Samples Panel
- plotting results against feature values (e.g., in analysis reports)
- effecting whether samples are used at all for modeling and analyses (see `Quality`)
- effecting how samples are used in calibration/classification (see `Usage`)
- providing reference values for calibration/classification and validation

- joining features from a loaded table with existing samples by means of a matching key feature

Sample File and Data Table File

Both, sample files and data table files are physical files on the hard disk. Sample files contain xy-data of one or multiple samples and are typically generated by measurement software. Data table files contain references to sample files plus optional sample features and are typically created by the user, either with PEAXACT or with Excel.

Getting Access to Samples

The Samples Panel can be used to select a sample and then get displayed additional information about it in the Properties Panel.

3.4.2 Load Sample Files

Toolbar:	
Menu bar:	Data > Load Samples...
Hot key:	CTRL + L
Context menu:	Samples Panel > Load Samples...
Context menu:	Model Tree > Hard Model Item > Load Underlying Sample
Drag & drop:	from Explorer to Samples Panel

Loads sample spectrum files. A File Dialog can be used to browse directories and select one or more sample files to be loaded. Choose a file filter from the drop-down list to localize certain sample files.

PEAXACT loads all samples it finds in a sample file. URIs are created automatically from the filename and IDs of the samples within the file. See also Sample Files for further information about URIs.

A loaded sample gets added to the Samples Panel if

- it is new, i.e., none of the already loaded samples has the same URI
- in case of OPUS-files, the block name matches the block name filter (see preferences)

Drag and Drop

A fast way to load sample files is by using drag & drop. Drag files from the Windows Explorer (e.g.) and drop them into the Samples Panel. Hint: If your directory contains many different files, you can simply select all files and drop them to the Samples Panel. PEAXACT automatically filters out sample files. You may also drag & drop directories to load all sample files and data table files from the directory.

3.4.3 Load Data Tables

Toolbar:	
Menu bar:	Data > Load Table…
Hot key:	CTRL + T
Drag & drop:	from Explorer to Samples Panel

Loads data table files. A File Dialog can be used to browse directories and select data table files to be loaded.

PEAXACT loads all samples it finds in a data table file. URIs are taken as is from the first table column, feature values are taken from other table columns.

A loaded sample gets added to the Samples Panel if it is new, i.e., none of the already loaded samples has the same URI. Otherwise, features of the loaded sample get merged with the existing sample.

Drag and Drop

A fast way to load data tables is by using drag & drop. Drag files from the Windows Explorer (e.g.) and drop them into the Samples Panel. You may also drag & drop directories to load all sample files and data table files from the directory.

3.4.4 Unload Selected Samples

Menu bar:	Data > Unload Selected Samples
Hot key:	CTRL + U
Context menu:	Samples Panel > Unload Selection

Unloads selected samples and removes them from the Samples Panel. If the currently active sample gets removed the next available sample becomes active. Component Fits to removed samples are removed along with them.

3.4.5 Unload All

Menu bar:	Data > Unload All

Unloads all samples at once. This is a fast way to clear the Samples Panel. All Component Fits are removed as well.

3.4.6 Save Data Table

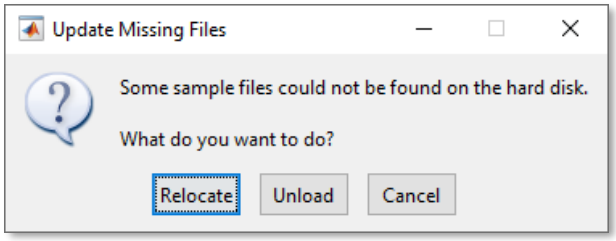
Menu bar:	Data > Save Data Table...
Menu bar:	Data > Data Inspector... > Data Table Editor >
Context menu:	Samples Panel > Save as Data Table...

Exports selected samples to a data table file. A File Dialog can be used to browse directories and select or enter a filename.

3.4.7 Update Missing Files

Menu bar:	Data > Update Missing Files
Samples Panel:	Activate a sample whose file is missing

Checks all samples for invalid URIs. If any are found, a dialog is shown which can be used to either relocate these files or unload affected samples.

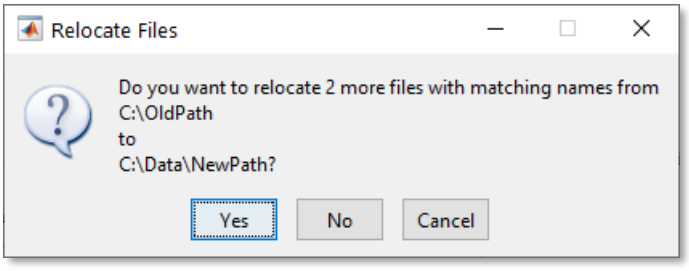


URIs become invalid if sample files get moved or renamed on the hard disk while being loaded in PEAXACT, or if a session file gets opened which contains samples that have been moved or renamed since the session was saved.

Relocate

Relocating comprises two steps:

- Relocating the next missing file, i.e., select a new target directory and target filename using the File Dialog.
- If possible, automatically relocating more missing files with matching names from the source directory to the selected target directory.



Note: Relocating sample files is fast and easy if files were only moved from one directory to another directory. Try to avoid moving sample files from one directory to many different directories. Also avoid renaming sample files.

Both steps execute until either all missing files are relocated or the user cancels.

Unload

Unloading removes all samples which are pointing to missing files.

3.4.8 Edit Samples

Editing samples refers to adding, removing, and modifying sample features. It is not possible to edit the sample spectrum (use models instead), or the sample file path (update missing files instead).

Edit Samples with PEAXACT

PEAXACT comes with its own integrated Data Table Editor which is part of the Data Inspector.

Menu bar:	Data > Data Inspector... > Data Table Editor
Menu bar:	Analysis > Data Inspector... > Data Table Editor
Context Menu:	Samples Panel > Data Inspector > Data Table Editor

In addition, the context menu of the Samples Panel offers shortcuts to changing the Quality and Usage features, and to fully removing all features. These actions are applied to selected samples.

Context Menu:	Samples Panel > Set Quality > ...
Context Menu:	Samples Panel > Set Usage > ...
Context Menu:	Samples Panel > Remove Features

Edit Samples with Microsoft Excel

Microsoft Excel can be used as an external editor for samples. You can use Excel to create and edit data table files and then load these data tables in PEAXACT. Because Excel is a powerful spreadsheet editor this is a convenient way to edit samples. However, keep in mind that you must load the data table file in PEAXACT to import changes made externally.

Consider the data table formatting rules when changing the table. Beside these rules you are free to use all Excel functionalities like formulas, diagrams, filters, conditional formatting, and so on.

Common practice

A typical procedure for editing samples involves creating an initial data table file with PEAXACT and then editing the file with Excel:

- Load sample files in PEAXACT

- Select samples in the Samples Panel and choose Data > Save Data Table from the menu. This creates a data table file that contains sample URIs only.
- Use Excel to edit the data table file (e.g., add concentrations)
- Load the final data table file in PEAXACT to import features to existing samples.

3.4.9 Sort Samples

Context Menu:	Samples Panel > Sort Selection by

Sorts and reorders selected samples in the Samples Panel. Samples can be sorted by name or any available sample feature.

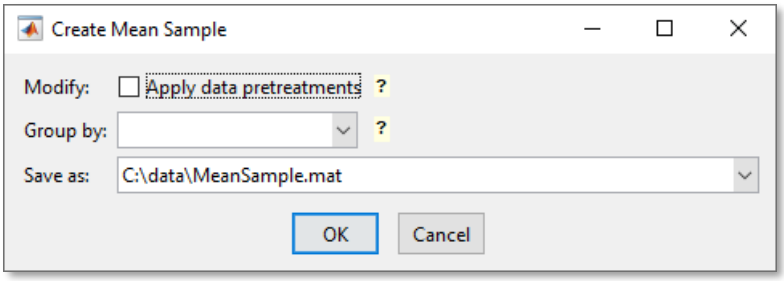
Sort order

Unsorted samples get sorted in ascending order (a to z, 0 to 9) when sorted once, and in descending order when sorted a second time. The sort order has no effect on any analysis results but sometimes on how the results are displayed.

3.4.10 Create Mean Sample

Menu bar:	Data > Create Mean Sample...

Creates and saves a mean sample from selected samples in the Samples Panel. At least 2 samples must be selected. The mean sample is created by averaging spectra and by copying feature values which are the same for all selected samples.



`Modify`

If a model is active, its Pretreatment Model can be applied to all selected samples before the mean spectrum is calculated. Tick **Apply data pretreatments** to use this option.

Note: Do not enable this option if you later intend to analyze the new sample by a model because this could produce unexpected results (double pretreatments).

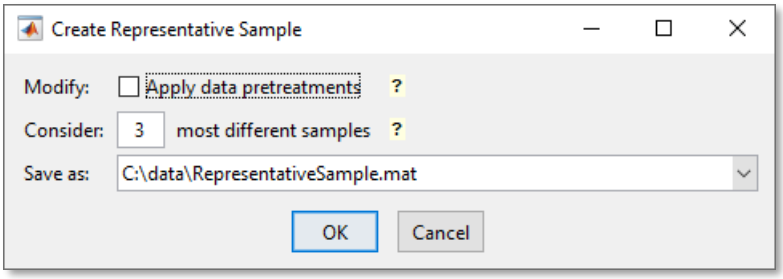
`Group by`	The optional grouping feature for group-wise creation of mean samples. Without grouping a single mean sample is created from all samples. If you choose a grouping feature, a separate mean sample is created for each group (group = samples having the same feature value). Samples with missing feature value are ignored. For example, you can use grouping to create a single mean sample for each group of repeated measurements.
`Save as`	The filename for saving the mean sample spectrum. If grouping is enabled, a separate file is saved for each group. The chosen filename automatically gets extended by the group name.

Click **OK** to create mean samples, save them to files, and add them to the Samples Panel.

3.4.11 Create Representative Sample

Menu bar:	Data > Create Representative Sample...

Creates a representative sample from selected samples in the Samples Panel. At least 2 samples must be selected. A representative sample is like a mean sample, but it is created from samples having the most different spectra among the selected samples. The representative sample spectrum typically will contain all peaks of all samples in a very pronounced manner. This makes it a suitable sample for creating a representative Hard Model for HMFA.



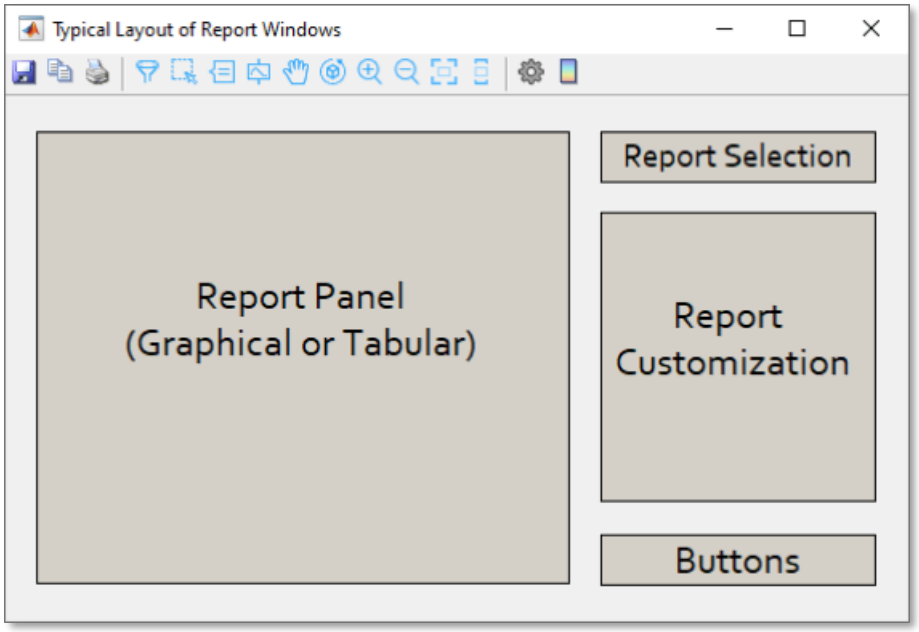
`Modify`	If a model is active, its Pretreatment Model can be applied to all selected samples before the mean spectrum is calculated. Tick **Apply data pretreatments** to use this option. Note: Do not enable this option if you later intend to analyze the new sample by a model because this could produce unexpected results (double pretreatments).

`Considered Samples`	The number of samples to consider for creating the representative sample. The algorithm will automatically pick the samples with most different spectra. The number should correspond to the number of chemical compounds in your measurements.
`Save as`	The filename for saving the representative spectrum.

Click **OK** to create the representative sample, save it to a file, and add it to the Samples Panel.

3.5 Reporting of Results

PEAXACT uses Report Windows to visualize results in graphical and tabular reports. All Report Windows have a similar layout and common functionalities which are explained in this section. Variations from the typical layout and custom functionalities are explained in separate sections dedicated to the individual Report Windows.



Typical Layout of Report Windows

Toolbar

	Export report as shown in the Report Panel to a file. Available file formats depend on the type of report, but in general, graphical reports can be exported to image files while tabular reports can be exported to text or spreadsheet files.

	Copy report to clipboard. Graphical reports are copied as rendered images or vector images (see preferences) while tabular reports are copied as text.
	Open the Print Preview Dialog.
	Data Filter Tool: enable to interactively edit Data Filters using the mouse.
	Data Cursor Tool: enable to read data directly from a graph by interactively placing Data Tips in a plot.
	Profile Cursor Tool (2D plots only): enable to display y-values of overlapping plots at a clicked x-position.
	Pan Tool (2D plots only): enable to interactively move the visible plot area with the mouse.
	Rotate Tool (3D plots only): enable to interactively rotate the orientation of a graph with the mouse.
	Zoom Tools (2D plots only): enable to interactively zoom in or out on a graph with the mouse.
	Full Zoom, Full Y-zoom
	Open Preferences Editor
	Show/Hide color bar

Note: The exact set of available toolbar icons depends on the specific Report Window. However, same icons have the same meaning each time.

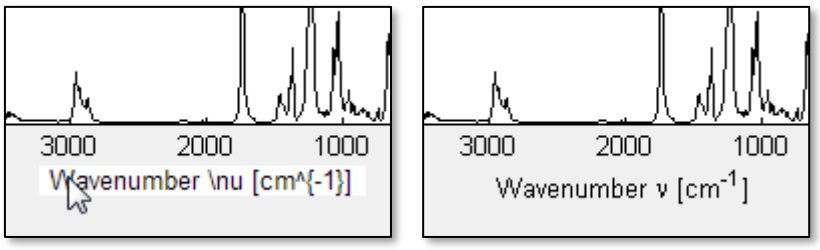
Report Selection & Customization

The report to be displayed in the Report Panel can be chosen from a drop-down list located at the top-right of the Report Window. Each individual Report Window has a very specific list of available reports.

Most reports can be customized in various ways using some controls located at the right of the window.

Changing Report Appearance
The appearance of reports (e.g., font size, visible elements of graphs) is controlled by several adjustable preferences. You can reach the Preferences Editor from the toolbar.

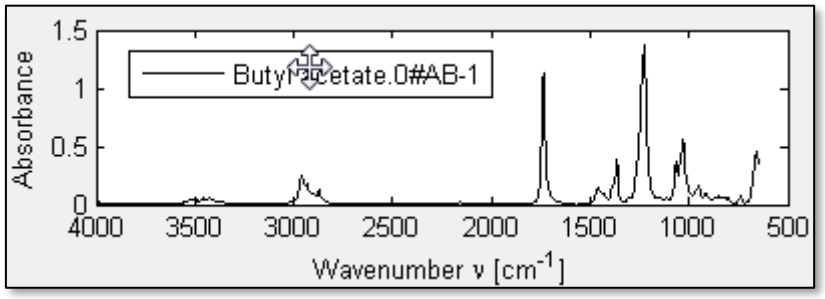
Editing Titles and Labels
All titles and labels of graphical reports can be edited when clicking on them.



Note that your text is processed by a TeX interpreter, i.e., you can use ^ for superscripts, _ for subscripts, {} for grouping. Also, you can use special commands for Greek letters (`\alpha`, `\beta`, `\gamma`, `\Gamma`, ...). When finished editing, press the Escape key, or click anywhere outside the text field.

> Note: User edited titles and labels are replaced by default text each time the selected report changes. Therefore, it is recommended to customize titles and labels as a final step before exporting the report to a file.

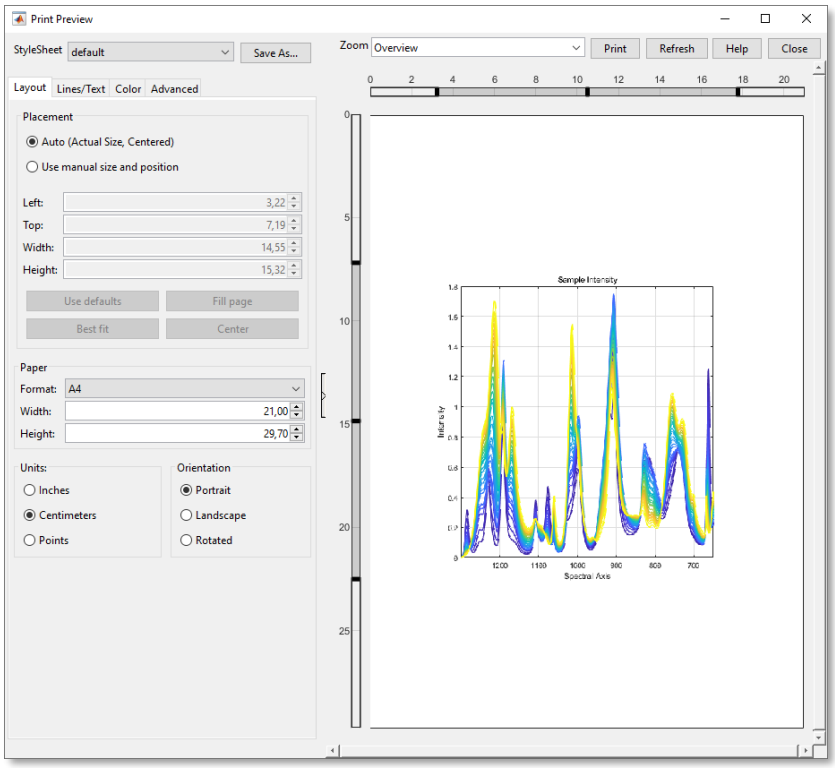
Positioning of Legends
Legends in graphical reports are positioned automatically to least interfere with the plots. However, you can reposition legends interactively by dragging them to the desired location.



Print Preview Dialog

The Print Preview is a dialog box showing the graphical report as it will print. A scaled version of the report displays in the right-hand pane of the window.

Use the Print Preview dialog box, shown below, to control the layout and appearance of graphical reports before sending them to a printer or print file.



3.6 Data Inspector

Menu bar:	Data > Data Inspector...
Menu bar:	Analysis > Data Inspector...
Context Menu:	Samples Panel > Data Inspector

The Data Inspector is a window designed for editing and visualizing samples. For this purpose, the Data Inspector consists of two parts:

- Data Table Editor for editing sample features
- Data Plotter for visualizing sample spectra and features in various 2D and 3D plots.

The Data Inspector does not require a model; it operates on samples alone. You typically use the Data Inspector to visually inspect sample spectra and manage features before you start with modeling.

To learn more about samples, see About Samples.

Opening the Data Inspector

When you open the Data Inspector, selected samples are imported from the Samples Panel into the Data Inspector. To import a separate set of samples, simply change the selection in the Samples Panel and open the Data Inspector again.

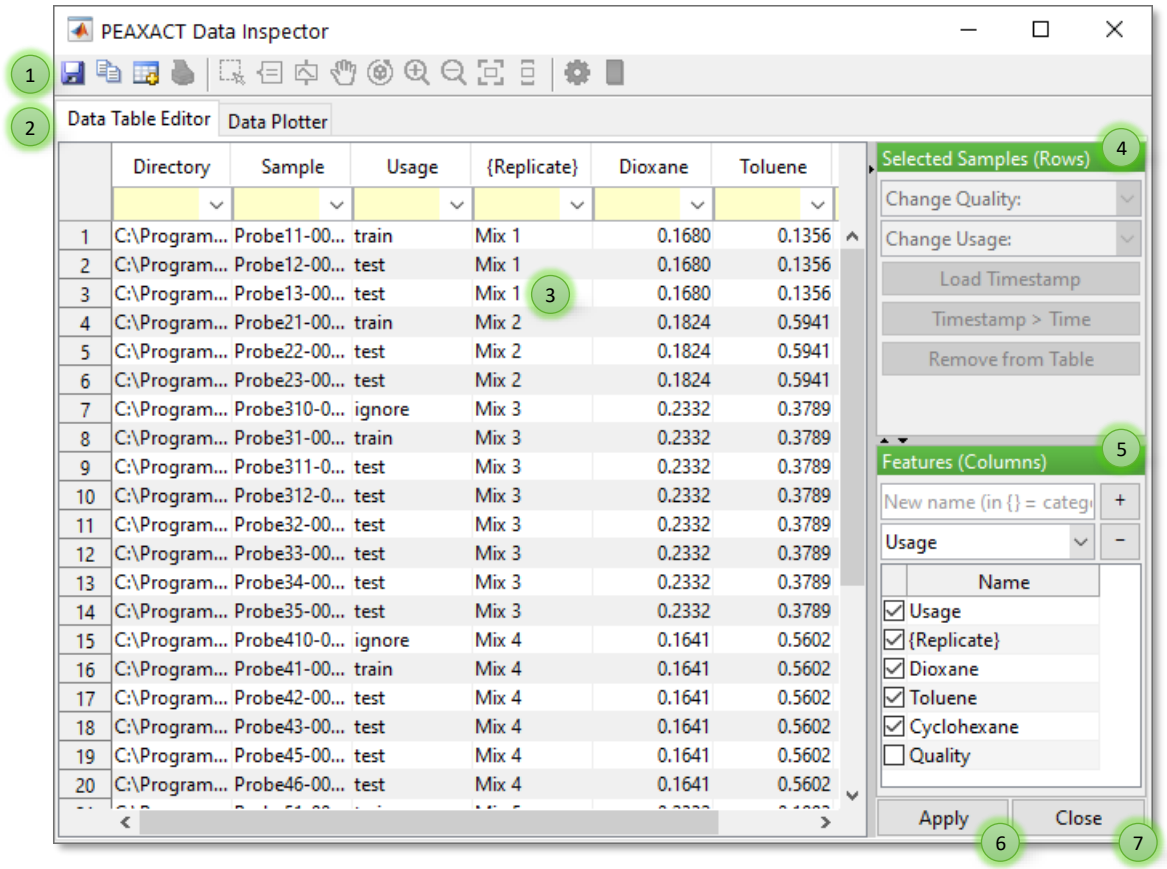
> Caution: Re-opening the Data Inspector refreshes its content. Unsaved changes made in the Data Table Editor will get lost.

Closing the Data Inspector

When you close the Data Inspector while the Data Table Editor has unsaved changes, you will be asked whether to apply changes. Doing so exports features back to the Samples Panel.

3.6.2 Data Table Editor

The Data Table Editor can be used to add, remove, and modify sample features. Each feature is represented by a table column. The first two columns are read-only; they contain the sample's directory and file name.



Data Inspector – Data Table Editor

1) Toolbar; see Report Window
2) Data Table Editor and Data Plotter tabs
3) Table with columns:
   - Directory: path of sample file (read-only)
   - Sample: sample name (read-only), printed in red if file is missing
   - any number of feature columns (editable)
4) Actions applicable to selected rows
5) Actions applicable to feature columns: add, remove, hide, show, rename
6) Apply button: accept table changes and update samples in the main window
7) Close button: close the Data Inspector window

Sort Rows
Rows can be sorted by clicking on a column header. Clicking multiple times toggles the sort order. Pressing the CTRL-key while clicking multiple column headers enables multi-level sorting.

Filter Rows
Rows can be filtered using the filter editor below the column header. Only rows matching the filter will be displayed. Choose a value from the drop-down list or enter the desired value into the text field. Filter expressions may contain wildcard characters to match any character, e.g., `3.1415*`

`*`	matches zero or more arbitrary characters.
`+`	matches one or more arbitrary characters.
`?`	matches exactly one arbitrary character.
Filter expressions may also be logical expressions, e.g., `> 0` or `<>ignore`.	
`>`	greater than filter
`>=`	greater or equal filter
`<`	less than filter
`<=`	less or equal filter
`=`	equal filter (exact match)
`<>`	not equal filter

Re-arrange Columns
Table columns can be re-arranged by dragging a column header and moving the column to the desired position.

Resize Columns
The width of a table column can be changed by dragging its border to the desired position. You can also auto-adjust the column width by double clicking the border.

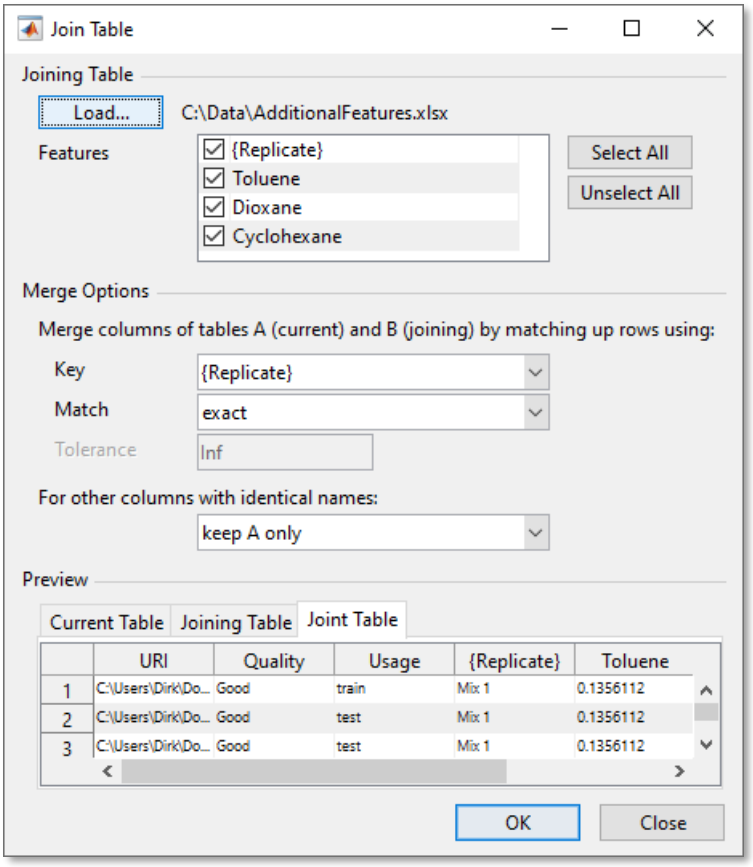
Export Options

Use the Export Tools  from the toolbar to export the table to a Data Table File or to the Windows clipboard, respectively. Columns `Directory` and `Sample` are combined and exported as a single column representing sample URIs. When exporting to a file, URIs pointing to subdirectories of the table file path are converted to relative paths. For more information about sample URIs see Sample Management.

Join Table

Use the Join Tool  from the toolbar to open the Join Table Dialog and join features of a second table with samples of the current table. The second table may or may not contain sample URIs

(see Data Table File for possible table file layouts). Features of the second table are merged with the current table either by matching URI, or row-by-row, or by a common feature.



`Load...`	Click to load a second table (joining table) which should be merged with the current table. Note: Joining tables will not add new rows (new samples) from the joining table to the current table. Only columns (features) will be merged. Use the PEAXACT main window if you want to load additional samples.
`Features`	The list displays all features available in the joining table. Select which features you want to merge with the current table.
`Select All / Unselect`	Click to select / unselect all features.

Merge Options

`Key`	The key property to be used for matching rows of the joining table with rows of the current table. The key must be a property which both tables have in common. The following options are available:

	`Sample URI`. Rows of the joining table are merged with rows of the current table for rows with identical URIs. Each row of the joining table is merged with zero or one row of the current table.
	`Row Index`. Rows of the joining table are merged with the current table row-by-row. If the joining table has more rows than the current table, additional rows are ignored.
	`Common feature`. Rows of the joining table are merged with rows of the current table according to the value of a common feature. You may specify additional match conditions, e.g., whether the key value must match exactly or may be within a tolerance.
`Match`	The option for how key values are matched. The following options are available:
	`exact`. Each row of the joining table is merged with all rows of the current table where the key matches exactly.
	`closest`. Each row of the joining table is merged with the one row of the current table where the key is the closest match within the specified `Tolerance` (see below).
	`closest below`. Each row of the joining table is merged with the one row of the current table where the key value of the joining table is closest below the key value of the current table.
	`closest above`. Each row of the joining table is merged with the one row of the current table where the key value of the joining table is closest above the key value of the current table.
	`all within tolerance`. Each row of the joining table is merged with all rows of the current table where the key value is within the specified `Tolerance` (see below).
	`case-insensitive`. Each row of the joining table is merged with all rows of the current table where the key matches exactly except for the case. Available only for categorical keys.
`Tolerance`	The tolerance for the matching of numerical key values. The tolerance value can be `Inf` (= infinite) which effectively deactivates the tolerance so that there will always be at least one match. For a non-Inf tolerance it may also happen that no key matches.
`Tolerance Unit`	The unit of the tolerance value. Available only when `Key = Timestamp`.

`Columns with identical names`	Specifies how a column of the joining table (B) should be treated if the current table (A) has a column with same name. The following options are available:
	`keep A only`. The column of the joining table is ignored.
	`merge - fill empty cells of A with B`. Values of the current table are not changed; empty cells are filled with values of the joining table.
	`merge - fill empty cells of B with A`. Values of the joining table overwrite values of the current table; empty cells of the joining table are ignored.
	`keep B only`. The column of the joining table replaces the column of the current table.

Preview
Use the preview table to see whether the result is as expected. Click **OK** to accept the joint table.

Edit Feature Values

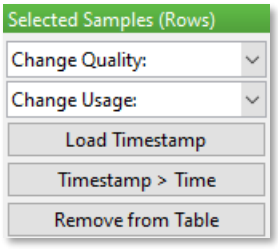
Edit the table by clicking into a table cell and modifying the value. Use the Enter (Escape) key to accept (discard) your changes. Press the Tab key or the arrow keys to accept changes and move the cursor to an adjacent cell. You can use the cut/copy/paste/delete keys to manipulate the table.

> Note: Changing the table does not yet change the underlying samples. You must click the Apply button to update samples in the main window.

Columns `Directory` (sample path) and `Sample` (sample name) are read-only. All other columns are editable. The possible value for each feature depends on whether it is a numerical, categorical, or special feature. See About Samples to learn more about features.

Edit Selected Samples

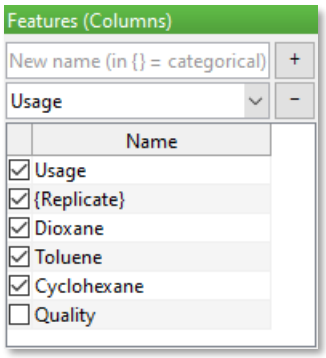
From the top-right panel of the Data Table Editor you can apply some actions to all selected samples (table rows). A row counts as selected if any cell in the row is selected.



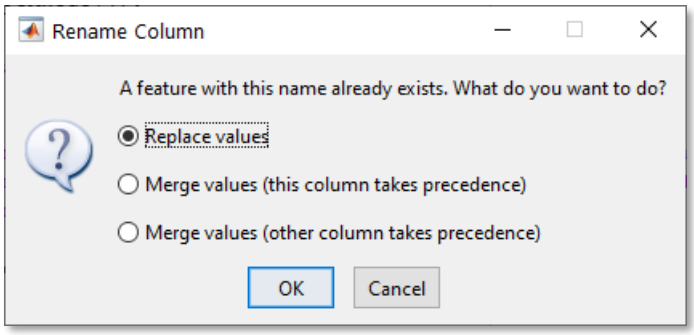
`Change Quality`	Select a value from the drop-down list to assign the value to all selected rows.
`Change Usage`	Select a value from the drop-down list to assign the value to all selected rows.
`Load Timestamp`	Click to automatically assign the value of the `Timestamp` column. The column is added if missing. Existing values will be overwritten. The value is read from the sample file content if possible, or from the file system otherwise.
`Convert Timestamp to Time`	Click to convert values of column `Timestamp` (if available) to relative time values. A dialog opens which allows you to select a reference timestamp for time = 0 and a time unit. All time values will be calculated relative to the reference timestamp.
`Remove from Table`	Click to remove all selected rows from the table. Note that removing table rows does not remove samples from the Samples Panel (main window) but just from the Data Inspector.

Edit Features

From the bottom-right panel of the Data Table Editor you can perform actions to modify features (table columns).



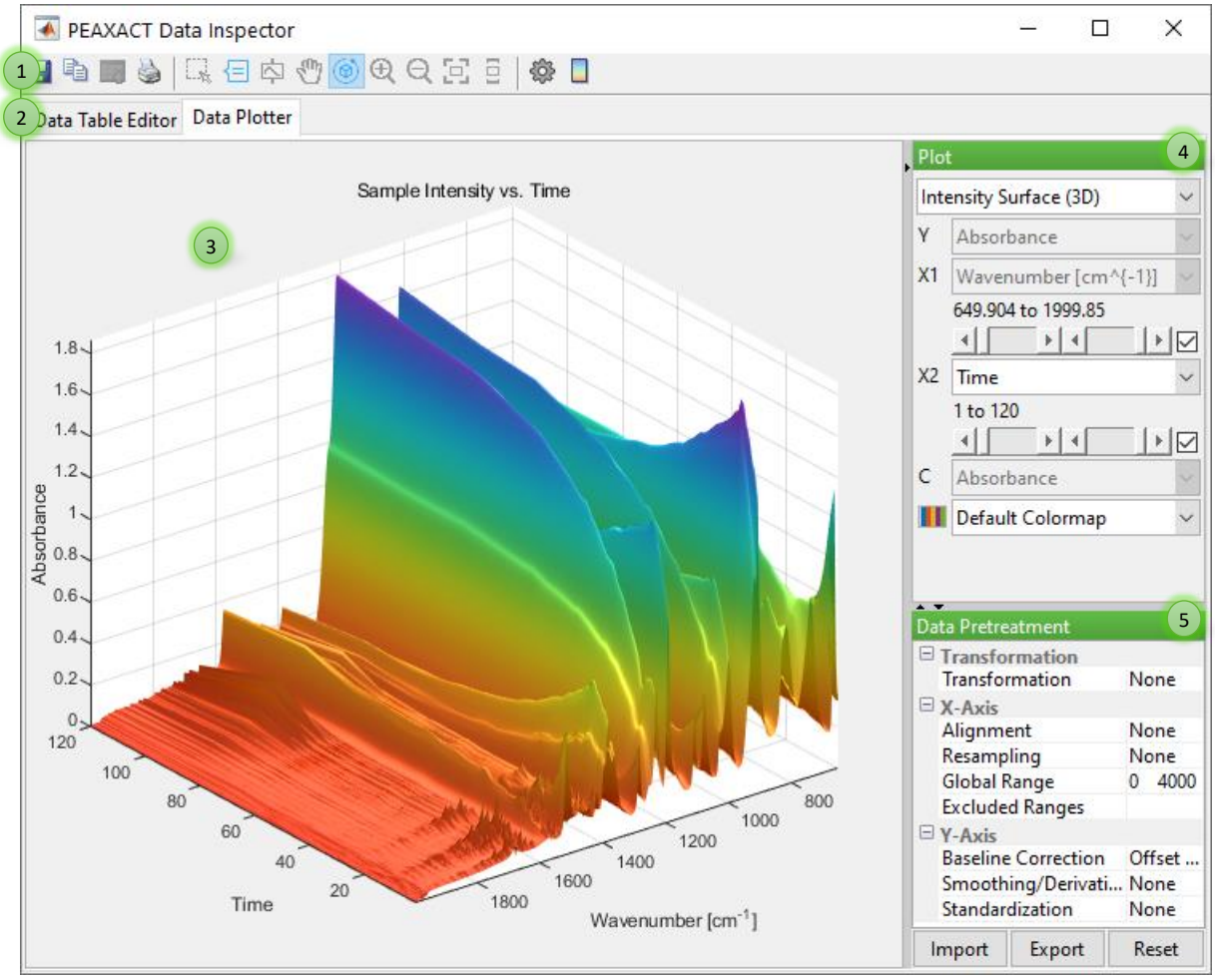
`Add feature`	Enter the new feature name in the text field and press the **[+]** button. You can enter regular or special feature names. Put the name in braces to make the feature categorical. The name is added to the feature list and a new column is added to the table. Names of regular features are case-sensitive; names of special features are not; See About Samples for a list of special feature names. If you enter a special feature name it is automatically converted to upper case syntax (e.g., `Timestamp` instead of `timestamp`).

`Remove feature`	Select a feature from the drop-down list and press the **[-]** button to delete the feature. The corresponding column will be removed from the table and from the feature list.
`Show / Hide feature`	Tick or untick the checkbox of a feature in the feature list to show or hide it. Hiding a feature temporarily removes it from the table and from graphical plots.
`Rename feature`	Use the feature list to edit the name if visible or hidden features. You can put a name in curly braces to convert a numerical feature to a categorical feature. Be careful when removing curly braces from feature names because categorical values cannot be converted back to numerical values. Feature names must be unique. If you rename a feature to another name in the list, you must decide whether to replace or merge column values:  Note: `Quality` and `Usage` are reserved names. You can neither rename those features nor rename any other feature to a reserved name.

3.6.3 Data Plotter

The Data Plotter generates customizable graphical reports of sample spectra and features.

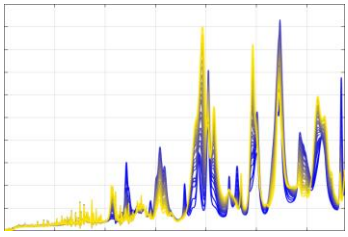
The layout of the Data Plotter matches the typical layout of a Report Window (see for a description of functionalities common to all Report Windows). This section focuses on specifics of the Data Plotter Window.



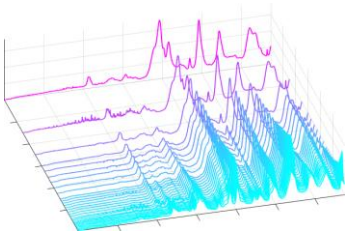
Data Inspector – Data Plotter

1) Toolbar
2) Data Table Editor and Data Plotter tabs
3) Report Panel
4) Plot Selection Panel
5) Data Pretreatment Panel

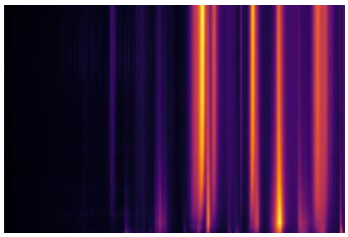
Available Reports



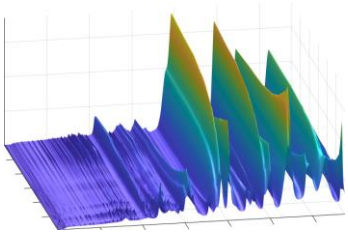
Samples (2D)
Plot of sample spectra.
y-axis: signal intensity
x-axis: spectral axis
colored by: selectable feature



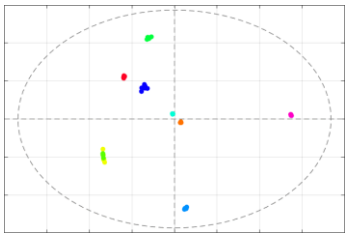
Samples (3D)
Plot of sample spectra, arranged along the x2-axis.
y-axis: signal Intensity
x1-axis: spectral axis
x2-axis: selectable feature
colored by: selectable feature



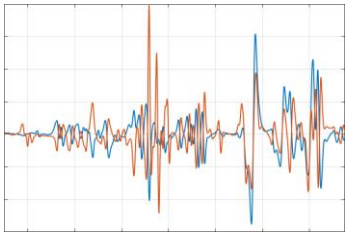
Intensity Surface (2D)
Heat map of signal intensities.
x1-axis: spectral axis
x2-axis: selectable feature
colored by: signal intensity



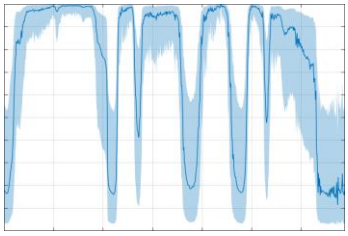
Intensity Surface (3D)
Surface plot of signal intensities.
y-axis: signal intensity
x1-axis spectral axis
x2-axis: selectable feature
colored by: signal intensity



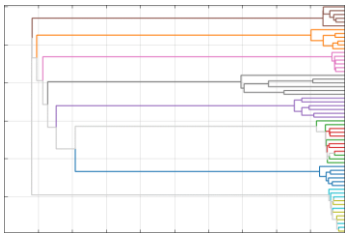
PCA Scores
Principal component (PC) scores.
x-axis: score on a selectable PC
y-axis: selectable feature or another score on selectable PC
colored by: selectable feature



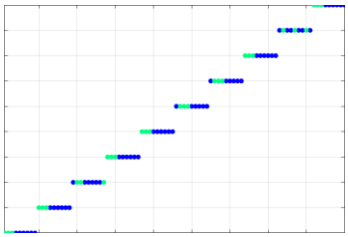
PCA Loadings
Principal component (PC) loadings.
y-axis: loadings on a selectable PCs
x-axis: spectral axis
colored by: sequence



Correlation Plot
Correlation of signal intensities with a selectable feature.
y-axis: correlation in % with a selectable feature
x-axis: spectral axis



Clusters (Dendrogram)
Hierarchical cluster tree representing the distance between sample spectra.
y-axis: each tree leaf represents a sample
x-axis: distance measure between samples
colored by: selectable feature

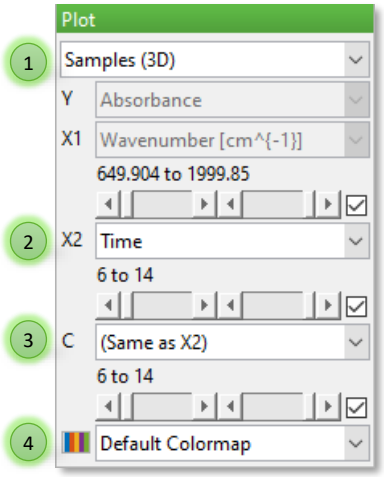


Features
Plot of any two sample features.
y-axis: selectable feature
x-axis: selectable feature
colored by: selectable feature

Report Customization

Plot Configuration

The Plot Configuration Panel of the Data Plotter contains controls for changing axis variables and colors.

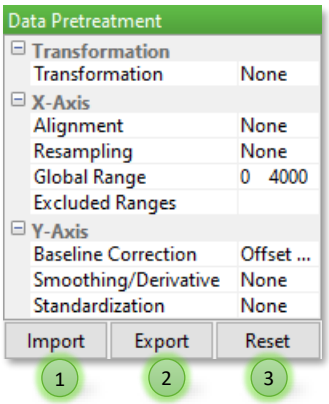


1) Select a report.
2) If available, choose variables for the x-axis and y-axis. Use the sliders to change the visible range of values. Use the checkbox to enable/disable the effect of the sliders.
3) If available, choose a variable for coloration of the plot.
4) Choose a color scheme. The default colormap depends on the selected report and for some reports also on the selected axis variables.

Note: The actual number of visible and editable configuration controls depends on the chosen report.

Data Pretreatment

The Data Pretreatment Panel of the Data Plotter contains controls for data manipulations. The impact of these settings can directly be previewed in the Report Panel.



1) Import Pretreatment Model from active model (main window).
2) Export to Pretreatment Model of the active model or to new model.
3) Reset to default Pretreatment Model of the active session profile.

Pretreatment settings used by the Data Plotter have the same meaning as in the Pretreatment Model. However, the Data Plotter keeps its own instance of settings. You can exchange settings between the Data Plotter and the active model by using the Import (1) and Export (2) buttons. On export you can also choose to create a new model.

3.7 Modeling

Modeling is the process of creating a model for analyzing samples. It is subject to the specifics of a chosen analysis method. For instance, modeling for peak integration comprises the definition of an Integration Model, while ***Spectral Hard Modeling*** comprises the creation of a Hard Model.

This section explains modeling functionalities of PEAXACT. See section Analysis to learn more about how to use the model for analysis.

3.7.1 Model

The term *model* (without predicate) typically refers to the top-level model container that consists of sub-models and that can be saved to a model file. In contrast, sub-models are referred to by predicates, e.g., Pretreatment Model.

Modification

Properties Panel: Click Model Tree > Model Item

A model contains a few top-level properties that can be modified with the Model Properties Panel:

`Description`	A free text to describe the model or provide additional information.

`Report Directory`	The suggested default directory for saving reports (e.g., analysis results). The directory can be specified as absolute path (starting with a drive letter or double slash) or relative path. The latter will be resolved to a path relative to the model's directory. For more details see Report File.

See the following section for how to modify the sub-models.

Undo & Redo

Menu bar:	Edit Model > Undo / Redo
Hot key:	CTRL + Z / CTRL + Y

Each model keeps a history of its most recent changes (see preferences). You can undo and redo these modifications step-by-step.

Undo/Redo is model-specific, i.e., each model has its own history.

3.7.2 Pretreatment Model

The Pretreatment Model is a sub-model that provides options for manipulating the sample signal. Pretreatments defined by different models never interfere because only the active model's Pretreatments Model manipulated the sample signal, and only temporarily while the model is active.

The Pretreatment Model also stores a collection of user-defined Data Filters. A Data Filter specifies regions of the sample signal to be used for later operations. The filter only gets applied when used in an operation, e.g., during PLS calibration. Otherwise, Data Filters are inactive and have no effect. When active though, Data Filters are applied independent from each other to the pretreated sample signal, i.e., after all other pretreatments have been carried out.

Pretreatments are carried out before all other operations in the following order:

- Transformation
- NMR-specific processing
- Alignment
- Resampling
- Reduction to Global Range
- Baseline Correction
- Smoothing / Derivatives
- Standardization
- Removal of Excluded Ranges

Transformation

`Transformation`	The option for transforming the signal.
	`None`. Disabled
	`Transmittance > Absorbance`. Converts transmission to absorbance spectra. $Ab = -\log(Tr)$
	`% Transmittance > Absorbance`. Converts relative transmission (given in percent) to absorbance spectra. $Ab = -\log(Tr/100)$
	`NMR FID Processing`. Applies apodization and zero filling to NMR FIDs.
	`NMR FID > Spectrum`. Converts NMR FIDs to spectra using parameters `Spectrometer Frequency (MHz)` to convert between time and frequency domains, `Frequency Shift Mode` to specify a reference point for the frequency axis (`Offset` or `Center`), and `Frequency Shift (ppm)` to specify the x-value of the reference point. If enabled, apodization and zero filling are applied to FID, and phase correction is applied to the spectrum.
	`NMR FID > Spectrum (mirrored)`. Same as `NMR FID > Spectrum`, but the spectrum is mirrored horizontally.
	`NMR Spectrum Processing`. Applies apodization, zero filling, and phase correction to NMR spectra. Because some operations take place in the time domain, the `Spectrometer Frequency (MHz)` must be specified to convert between frequency and time domains.
`NMR Apodization`	The option for apodization of NMR FIDs.
	`None`. Disabled
	`Exponential`. Exponential apodization using the additional parameter `Exponential (Hz)` for the exponential apodization function.
	`Gaussian`. Gaussian apodization using the additional parameter `Gaussian (Hz)` for the Gaussian apodization function.
	`Exponential and Gaussian`. A combination of both exponential and Gaussian apodization.

NMR Zero Filling	The option for zero filling NMR FIDs to a specified size. The option has no effect if the initial FID size already exceeds the specified size.
	None. Disabled
	1024 (1k), …, 1048576 (1024k). The total number of data points after adding zeros.
NMR Phase Correction	The option for phase correction of NMR spectra.
	None. Disabled
	Manual. Manual phase correction using parameters for the Zeroth Order and First Order phase in degrees.
	Auto (Negative Peak Penalization). Automatic adjustment of zeroth order and first order phases by an algorithm which minimizes negative parts of the mean centered spectrum.

Modification of X-Values

Alignment	The option for aligning the x-axis with a reference.
	None. Disabled
	Reference Peak. Finds the x-position of the largest y-value within a specified Reference Peak Range and shifts the x-axis to align the reference peak with a specified Target Position.
Resampling	The option for changing the x-resolution by either removing data points or by recalculating y-values at new x-values.
	None. Disabled
	Thinning. Reduces the number of data points. For a specified Thinning Factor of N, every N^{th} data point is kept. N can be any decimal number greater than or equal to 1.
	Equidistant Points. Resamples data at a specified number of new x-values. For a specified Number of Points of N, y-values are recalculated at N equally spaced x-values within the visible range by linear interpolation.
	Reference Axis. Resamples data at new x-values loaded from a specified sample Reference File. Y-values are recalculated at the x-values of the reference sample by linear interpolation.

`Global Range`	The global range defines the smallest and largest x-value. Only signal in between is considered for analysis. This is useful for cutting off unwanted signal at the edges.
`Excluded Ranges`	Excluded ranges are defined by a lower and upper x-value. Signal in between is not considered for analysis. This is useful for cutting off local signal artifacts.

Modification of Y-Values

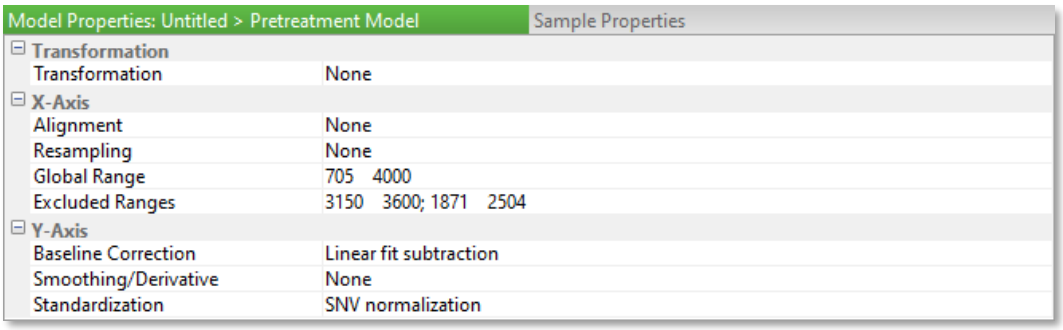
`Baseline Correction`	The option to subtract background signal.
	`None`. Disabled
	`Offset subtraction`. Subtracts a constant value such that the smallest value within the reduced spectral range is shifted to zero.
	`Straight line subtraction`. Subtracts a straight line from the left-most to the right-most data point within the reduced spectral range.
	`Linear fit subtraction`. Subtracts the straight line that is fitted best from below to the signal within the reduced spectral range.
	`Rubber band subtraction`. Fits a convex envelope to the spectrum's underside within the full spectral range. You can specify optional `Baseline Nodes` to mark points of the signal as baseline points. The outer left and right points are nodes by default, as well as each point at the edge of an excluded region. Add more nodes, e.g., to fit the baseline tighter to a concave part of the signal.
`Smoothing / Derivatives`	The option for smoothing and differentiating the signal to remove noise or separate overlapping signals.
	`None`. Disabled
	`Smoothing only`. Removal of noise by smoothing the signal. A `Smoothing Filter` must be specified that is the number of adjacent data points used for smoothing the central point. The greater the value, the smoother the signal. Note: If you have problems getting your data smoothed sufficiently even with the maximum filter length, consider using data thinning or other resampling options to reduce the total number of data points.

	`1st order derivative`. Numerical first derivation. Inflection points in the original signal are resolved to peaks. A `Smoothing Filter` must be specified (see above).
	`2nd order derivative`. Numerical second derivation. Shoulders of overlapping peaks in the original signal are resolved to peaks. A `Smoothing Filter` must be specified (see above).
`Standardization`	The option for scaling and shifting the signal.
	`None`. Disabled
	`Min-Max normalization`. Shifts the minimum y-value to 0 and scales the maximum y-value to 1.
	`Area normalization`. Shifts the y-center to 0 and scales y-values to a mean absolute deviation of 1.
	`SNV normalization`. Shifts the y-center to 0 and scales y-values to a standard normal variate of 1.
	`Peak normalization`. Scales y-values to a specified `Reference Peak Value` which is either the `Maximum` or the `Area` of a reference peak. The reference peak is defined by the following properties: `Reference Peak Range`: The lower and upper bound of the x-region of the reference peak. The peak value is calculated from data within this region. `Reference Peak Baseline`: The baseline type of the reference peak. For some types you can specify optional baseline ranges. `Lower Baseline Range`: The lower and upper bound of the lower x-region that is used to find the baseline. `Upper Baseline Range`: The lower and upper bound of the upper x-region that is used to find the baseline.

3.7.2.2 Modify Pretreatments

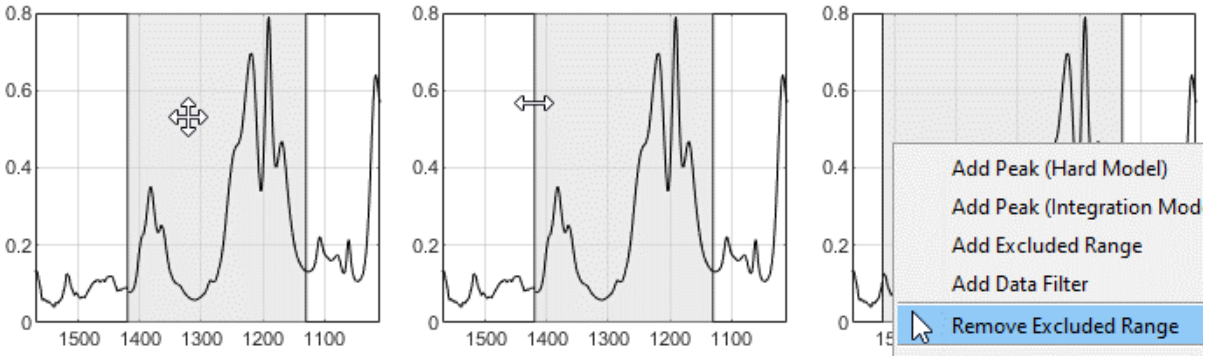
Properties Panel: Click Model Tree > Data Pretreatment Item

The Pretreatment Model can be modified by using the Model Properties Panel.



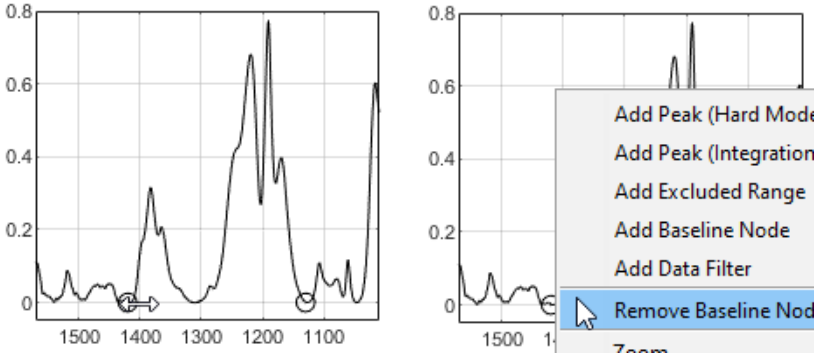
Interactive Modification of Excluded Ranges

New excluded ranges can be added via the context menu of the Plot Panel. Use the mouse to interactively modify bounds of excluded ranges (see preferences). Drag the gray area with the left mouse button to shift the whole range. Drag the boundary line to modify the boundaries. Right-click the area to open the context menu for more options.



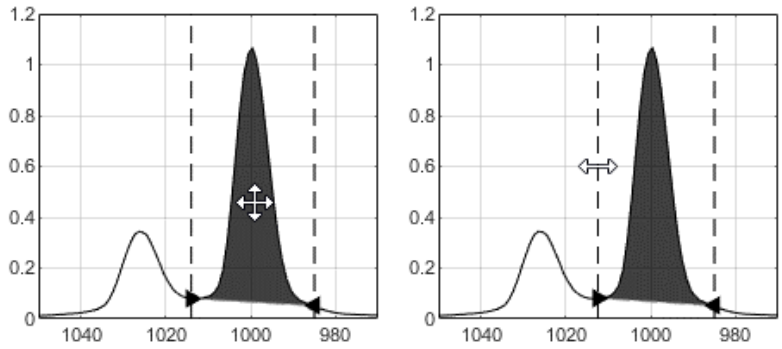
Interactive Modification of Rubber Band Baseline Nodes

If `Baseline Correction` is set to `Rubber Band Subtraction`, new baseline nodes can be added via the context menu of the Plot Panel. Use the mouse to modify baseline nodes. Drag the black circle with the left mouse button to shift the position of the node. Right-click the circle to open the context menu for more options.



Interactive Modification of Reference Peak for Normalization

If `Standardization` is set to `Peak Normalization`, the reference peak for normalization is displayed in the Plot Panel. Use the mouse to modify the reference peak. Drag the colored area with the left mouse button to shift the whole peak. Drag the vertical dashed lines or the arrows to modify the left or right boundaries. Drag the dotted lines (if available) to modify the left or right baseline regions. Hold the SHIFT key and drag the dash-dotted lines (if available) to create baseline regions.



3.7.2.3 Reset to Defaults

Menu bar:	Edit Model > Pretreatment Model > Reset
Context Menu:	Model Tree > Pretreatment Item > Reset

Resets the Pretreatment Model to defaults defined in the active session profile. This does not affect Data Filters.

3.7.2.4 Add Data Filter

Menu bar:	Edit Model > Pretreatment Model > Add Data Filter...
Context Menu:	Model Tree > Pretreatment Item > Add Data Filter...
Context Menu:	Plot Panel > Add Data Filter

Adds a new Data Filter to the Pretreatment Model. A dialog gets shown to specify the name of the new filter. Data Filters can get any name if it is unique within the Pretreatment Model.

A Data Filter added this way has no ranges specified. Modify the ranges, either manually using the Properties Panel, or interactively using the Data Filter Tool.

Adding Data Filters via Plot Panel

Context Menu:	Plot Panel > Add Data Filter

Right-click at the desired position in the Plot Panel and select **Add Data Filter** from the context menu. The new Data Filter gets a default name and has one range specified around the clicked point.

Modify the ranges, either manually using the Properties Panel, or interactively using the Data Filter Tool.

Adding Data Filters via Data Filter Tool

Toolbar:	

Enable the Data Filter Tool and make sure that no existing Data Filter is selected in the Model Tree Panel. Left-click at the desired position in the Plot Panel and move the mouse while holding the mouse button pressed. This adds a new Data Filter with default name.

3.7.2.5 Rename Data Filter

Menu bar:	Edit Model > Pretreatment Model > Rename Data Filter...
Context Menu:	Model Tree > Data Filter Item > Rename...

Renames the selected Data Filter. Data Filters can get any name if it is unique within the Pretreatment Model.

3.7.2.6 Remove Data Filter

Menu bar:	Edit Model > Pretreatment Model > Remove Data Filter
Context menu:	Model Tree > Data Filter Item > Remove
Context menu:	Plot Panel > Data Filter Item > Remove

Removes the selected Data Filter.

Removing Data Filters may affect other model elements which depend on them, e.g., the Calibration Model.

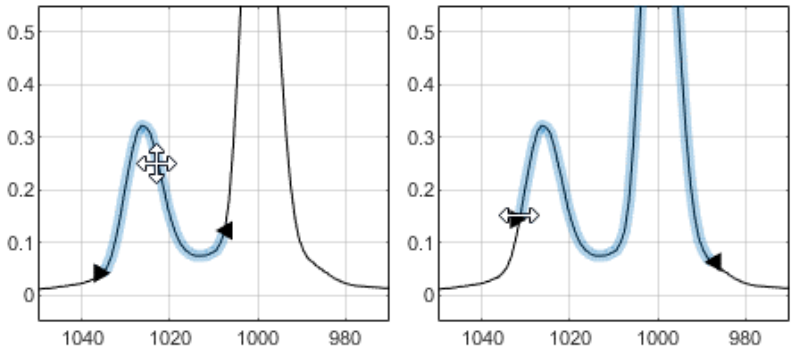
3.7.2.7 Modify Data Filter

Changing Parameter Values

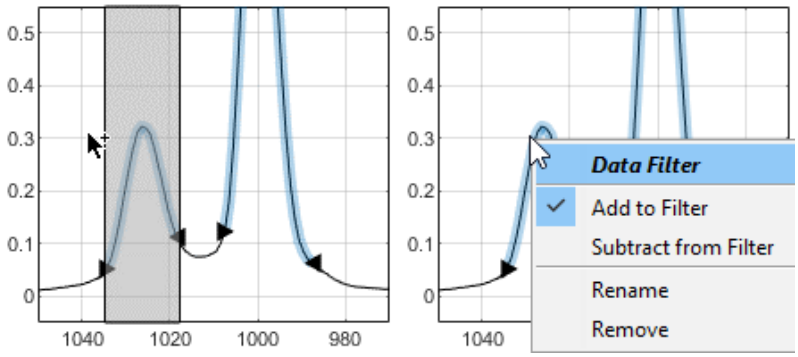
Select the Data Filter item in the Model Tree Panel to display the element's parameters in the Properties Panel. Use the table in the Properties Panel to change parameter values.

Modifying Data Filters Interactively

In the Plot Panel you can use the mouse to interactively modify ranges of the selected Data Filter. Drag a highlighted line segment with the left mouse button to shift the range. Drag the arrows to modify the left or right range boundary.



Enable the Data Filter Tool to get more modification options. Left-click and drag the mouse while the button is pressed to add or subtract ranges. Right-click to open the context menu for more options, e.g., toggle between add and subtract mode.



3.7.3 Integration Model

The Integration Model is a sub-model that consists of components, each containing one or more peaks specifying integration limits and a baseline for calculating the area under the sample signal.

Integration models can be utilized for Integration and, when combined with a Calibration Model, for Prediction.

3.7.3.1 Remove Integration Model

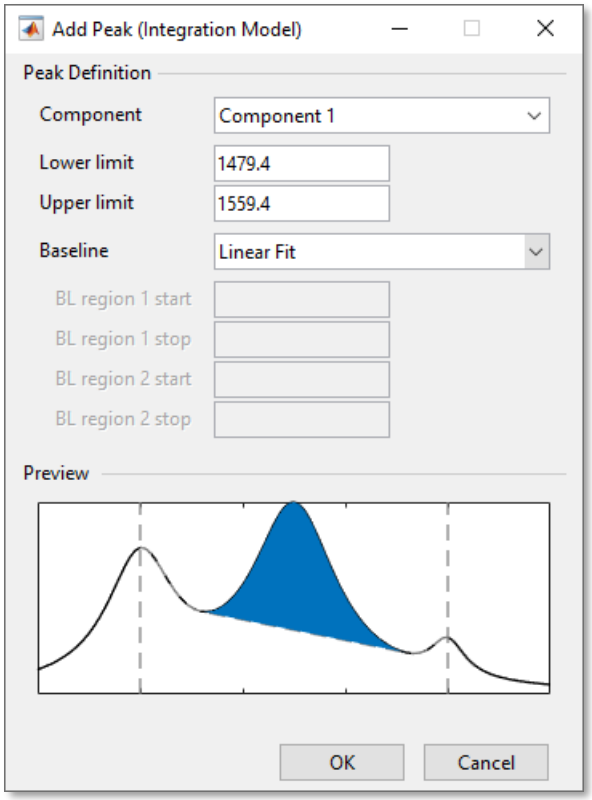
Menu bar:	Edit Model > Integration Model > Remove
Context menu:	Model Tree > Integration Model Item> Remove

Removes the whole Integration Model. Removing the Integration Model may affect other model elements which depend on it, e.g., the Calibration Model or Custom Results.

3.7.3.2 Add Peak

Toolbar:	
Menu bar:	Edit Model > Integration Model > Add Peak...
Context menu:	Model Tree > Integration Model Item > Add Peak...

Adds a new Integration Model Peak to either an existing component or a new component of the active model. A dialog gets shown to specify properties of the new peak.



`Component`	The component to which the peak should be added. Either select an existing component from the drop-down list or enter a new component name. Components can get any name if it is unique within the Integration Model.
`Lower/Upper limit`	X-values of the lower and upper integration limit.
`Baseline`	The type of the baseline to be subtracted from the signal. Some baseline types support the definition of separate baseline regions. The following baseline options are available:
	`None`. The baseline is zero. This option does not support baseline regions
	`Minimum Offset`. The baseline is a constant which is the *smaller* of the two values calculated from the left and right baseline regions. The calculated value is the mean signal (y-values) within each baseline region, or, for any unspecified region, the y-value at the closest integration limit.
	`Mean Offset`. Like `Minimum Offset`, but the constant is the *mean* of the two calculated values.

	`Straight Line`. The baseline is a straight line between two points calculated from the left and right baseline regions. The calculated points are the center (x-values) and mean signal (y-values) within each baseline region, or, for any unspecified region, the signal x- and y-values at the closest integration limit.
	`Linear Fit`. The baseline is a straight line fitted from below to the signal within the specified integration limits. However, the actual integration limits are then defined by the two points where the straight line touches the signal. This option does not support baseline regions.
`BL region 1 start/stop`	X-values of the region defining the left point of the baseline. Any empty value defaults to the lower integration limit.
`BL region 2 start/stop`	X-values of the region defining the right point of the baseline. Any empty value defaults to the upper integration limit.

Use the preview at the bottom of the dialog to evaluate your settings. Clicking OK adds the new peak to the Integration Model.

Adding peaks may affect other model elements which depend on the Integration Model, e.g., the Calibration Model or Custom Results.

Adding Peaks via Plot Panel

Context menu:	Plot Panel > Add Peak (Integration Model)

Right-click at the desired peak position in the Plot Panel and select **Add Peak (Integration Model)** from the context menu. The new peak has integration limits around the clicked point and a default baseline.

New peaks are added to the selected Integration Model Component, or, if no component is selected, to a new component with a default name.

3.7.3.3 Move Peak

Menu bar:	Edit Model > Integration Model > Move Peak to > ...
Context menu:	Model Tree > Integration Model Peak Item > Move to > ...
Context menu:	Plot Panel > Integration Model Peak Plot > Move to > ...

Moves the selected Integration Model Peak to either another component or to a new component. Choose the target component and, if it is a new component, enter the new component name. Components can get any name if it is unique within the Integration Model.

Moving peaks may affect other model elements which depend on the Integration Model, e.g., the Calibration Model or Custom Results.

3.7.3.4 Remove Peak

Menu bar:	Edit Model > Integration Model > Remove Peak
Context menu:	Model Tree > Integration Model Peak Item > Remove
Context menu:	Plot Panel > Integration Model Peak Plot > Remove

Removes the selected Integration Model Peak. You can remove any peak from any component and potentially leave empty components without peaks. Empty components always have a component area of zero.

Removing peaks may affect other model elements which depend on the Integration Model, e.g., the Calibration Model or Custom Results.

3.7.3.5 Rename Component

Menu bar:	Edit Model > Integration Model > Rename Component...
Context menu:	Model Tree > Integration Model Component Item > Rename...
Properties Panel:	Click Model Tree > Integration Model Item

Renames the selected Integration Model Component. Components can get any name if it is unique within the Integration Model.

3.7.3.6 Remove Component

Menu bar:	Edit Model > Integration Model > Remove Component
Context menu:	Model Tree > Integration Model Component Item > Remove

Removes the selected Integration Model Component. Removing components may affect other model elements which depend on the Integration Model, e.g., the Calibration Model or Custom Results.

3.7.3.7 Adjust Parameters

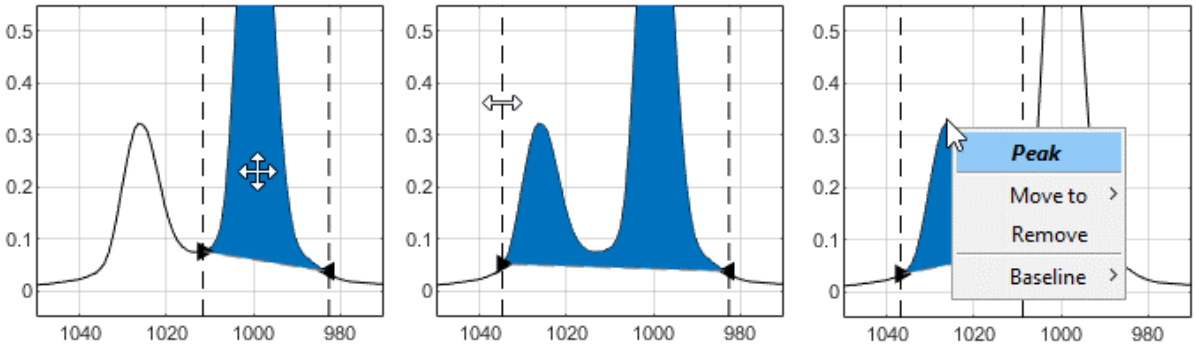
Changing Parameter Values

Select the Integration Model item in the Model Tree Panel or its graphical representation in the Plot Panel to display the element's parameters in the Properties Panel. Use the table in the Properties Panel to change parameter values.

Modifying Peaks Interactively

In the Plot Panel you can use the mouse to interactively modify the bounds of an Integration Model Peak. Drag the colored area with the left mouse button to shift the whole peak. Drag the

vertical dashed lines or the arrows to modify the left or right integration limits. Drag the dotted lines (if available) to modify the left or right baseline regions. Hold the SHIFT key and drag the dash-dotted lines (if available) to create baseline regions. Right-click the area to open the context menu for more options.



3.7.4 Hard Model

The Hard Model is a sub-model that consists of peak functions to represent a sample spectrum in a physically meaningful way. E.g., peak functions can overlap, shift, and change shape as observed in real spectra because of chemical and physical molecular interactions.

Hard Models can be utilized for Hard Modeling Factor Analysis, Component Fitting, and, when combined with a Calibration Model, for Prediction.

Nomenclature

When working with Hard Models, you should be familiar with the following wording:

Hard Model
A Hard Model in general is a mathematical function which is derived from equations representing the physics behind an underlying process. In PEAXACT, the term Hard Model refers to a function derived from the physics of molecular spectroscopy; it is a mathematical representation of a spectrum or a ***Spectral Hard Model***.

Physics tells us that a mixture spectrum is composed of superimposed peaks originating from the individual components in the mixture, with the components' concentrations being responsible for the peaks' intensities. This structural information is maintained in the Hard Model by means of a sum of peak-shaped curves. Subsets of peak-curves that represent pure component spectra are referred to as component models or Hard Model Components; they are multiplied by concentration-related weight parameters.

In summary, the Hard Model consists of weighted (Hard Model) Components which again consist of (Hard Model) Peaks. The Hard Model is completed by a simple baseline function.

Hard Model Component
The (Hard Model) Component is a mathematical representation of a pure component spectrum. It consists of (Hard Model) Peaks and has an associated component weight.

Hard Model Peak
The (Hard Model) Peak is a mathematical function with a peak-shaped profile. PEAXACT uses pseudo-Voigt functions. A pseudo-Voigt function is a linear combination of Gaussian and Lorentzian functions.

Component Weight
The component weight is the most important parameter of the Hard Model. Each Hard Model Component has an associated component weight parameter which represents the quantity of that component, i.e., component weights correspond to concentrations and therefore are relevant parameters for calibration. Component weights are determined automatically when fitting the Hard Model to samples.

Peak Parameters
Peak parameters are the parameters of Hard Model Peak, e.g., the position or width. Peak parameters can be set manually but are typically determined automatically by fitting the Hard Model to samples.

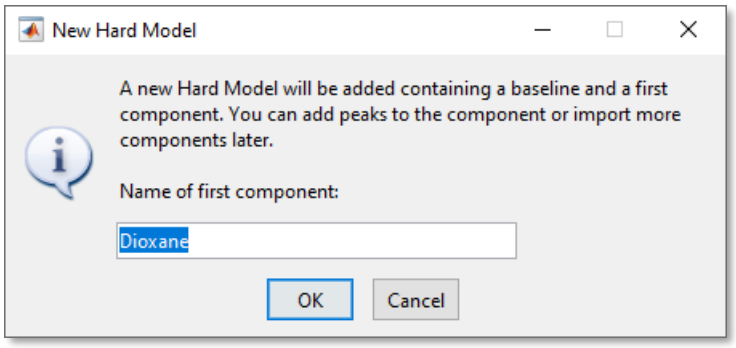
Editable Component & Editable Peaks
The first Hard Model Component is the *editable component* because peaks can only be added, removed, or modified in this component. Accordingly, peaks of the editable component are called *editable peaks*.

Model Fitting, Peak Fitting & Component Fitting
Model fitting is a general expression for a mathematical procedure in which the model's parameters are automatically adjusted until the model fits a certain measured spectrum. Peak fitting and component fitting are special kinds of model fitting which differ in the parameters being adjusted. Peak fitting refers to the adjustment of peak parameters of only the editable peaks. Component fitting mainly refers to the adjustment of component weights. Errors in component weights can be reduced by simultaneously adjusting peak parameters to account for peak variations in the measured spectrum. The extent of peak adjustments during component fitting is controlled by Hard Model settings.

3.7.4.2 New Hard Model

Menu bar:	Edit Model > Hard Model > New…
Context menu:	Model Tree > Hard Model Item > New

Adds a Hard Model to the active model. Use the dialog to specify the name of the first Hard Model Component. The first component of each Hard Model is also known as the editable component because new Hard Model Peaks can only be added, removed, and modified for this component.



Name of Editable Component

If your intention is to add peaks, consider naming the editable component after the pure component to be modeled. If you only intend to import other components, consider keeping the default name as the editable component is not relevant in this case. You can always rename components later.

If a sample is active while the new Hard Model is being created, the name of the editable component is suggested to be the sample name.

New Hard Model for Active Sample

Context menu:	Samples Panel > New Hard Model for Active Sample

When creating a Hard Model from the context menu of the Samples Panel the first component is automatically named after the active sample. If the currently active model already has a Hard Model, or if no model is active at all, a new model is created first.

New Hard Model If Required

Some hard modeling operations automatically prompt you to create a new Hard Model if none exists, e.g., when adding Hard Model Peaks or importing Hard Model Components.

3.7.4.3 Remove Hard Model

Menu bar:	Edit Model > Hard Model > Remove
Context menu:	Model Tree > Hard Model Item > Remove

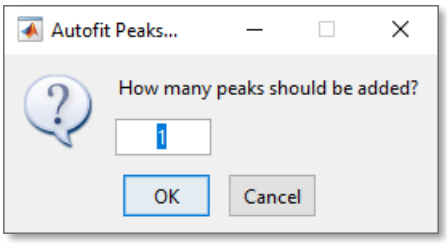
Removes the whole Hard Model. Removing the Hard Model also removes dependent elements such as Component Fits or the Calibration Model.

3.7.4.4 Add & Autofit Peaks

Toolbar:	
Menu bar:	Edit Model > Hard Model > Add & Autofit Peaks…
Context menu:	Model Tree > Hard Model Item > Add & Autofit Peaks…
Context menu:	Model Tree > First Component Item > Add & Autofit Peaks…

Auto-fitting of Hard Model Peaks is a combination of adding new peaks to the editable component and automatically adjusting editable peaks such that the model fits the active sample spectrum.

You are prompted to enter the number of new peaks. Start with a rough count of peaks in the sample and add more peaks later if required.



Note: New peaks will always be added to the editable component.

The peak fitting algorithm is controlled by model settings. In general, first the position of the next peak to be added is determined by analyzing the spectral residuals, then a new Hard Model Peak is added to the editable component, and finally the model is fitted to the active sample according to the peak fitting procedure.

3.7.4.5 Remove Selected Peaks

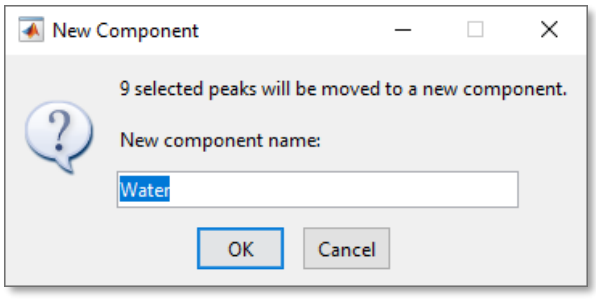
Menu bar:	Edit Model > Hard Model > Remove Selected Peaks
Context menu:	Model Tree > Hard Model Peak Item > Remove
Context menu:	Plot Panel > Hard Model Peak Plot > Remove

Removes selected peak from the editable component. You can also select a peak in the Model Tree Panel or its graphical representing in the Plot Panel and press the Delete key.

3.7.4.6 New Component from Selected Peaks

Menu bar:	Edit Model > Hard Model > New Component from Peaks…
Context menu:	Model Tree > Hard Model Peak Item > New Component…
Context menu:	Plot Panel > Hard Model Peak Plot > New Component…

Moves selected peaks from the editable component to a new component. You are prompted to enter the new component's name.



3.7.4.7 Import Components

Toolbar:	
Menu bar:	Edit Model > Hard Model > Import Components...
Context menu:	Model Tree > Hard Model Item > Import Components...
Drag & Drop:	from Explorer to Model Tree Panel

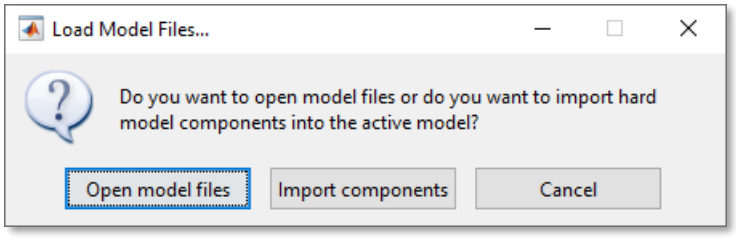
The File Dialog can be used to browse directories and select one or more model files to import Hard Model Components from. Choose a file filter from the drop-down list to localize certain model files. A model must be active to import components.

All non-empty components of the source models are copied to the active model. If no Hard Model exists yet, you will be prompted to create one first.

Names of imported components that already exist will automatically be numbered consecutively.

Drag and Drop

A fast way to import Hard Model Components is by using drag & drop. Activate the target model in the Model Tree Panel, then drag model files from the Windows Explorer, e.g., and drop them into the Model Tree Panel. You will be asked whether to open these files or to import components into the active model.



Component Equilibration

Imported Hard Model Component are equilibrated, which means that

- component weights are set to 1, and
- peak amplitudes of each component are scaled such that the maximum peak amplitude is in the same order of magnitude as the active sample (or 1 if no sample is active)

Component equilibration is reasonable because otherwise parameters of different components could have totally different orders of magnitude.

> Caution: Do not import components while a sample is active which is completely unrelated to the Hard Model.

3.7.4.8 Rename Components

Menu bar:	Edit Model > Hard Model > Rename Component...
Context menu:	Model Tree > Hard Model Component Item > Rename
Properties Panel:	Click Model Tree > Hard Model Item

Renames the selected Hard Model Component. Components can get any name if it is unique within the Hard Model.

3.7.4.9 Remove Components

Menu bar:	Edit Model > Hard Model > Remove Component
Context menu:	Model Tree > Hard Model Component Item > Remove

Removes the selected Hard Model Component. Removing components may affect other model elements which depend on the Hard Model, e.g., the Calibration Model or Custom Results.

> Note: You cannot remove the editable component.

3.7.4.10 Export Components

Menu bar:	Edit Model > Hard Model > Export Component
Context menu:	Model Tree > Hard Model Component Item > Export...

Exports the selected Hard Model Component to a new model file. The new model will contain a Hard Model with just the one component. In addition, the Pretreatment Model is copied to the new model too. The File Dialog can be used to browse directories and select or enter a filename for the model to be saved. By default, the component name is suggested as filename.

Exporting of components is not required if the Hard Model only contains a single component. In that case, simply save the model.

Overwriting Existing Files

As a precaution, you cannot save the model to a file of another model that is currently opened in PEAXACT. You must close the other model before overwriting its file.

3.7.4.11 Adjust Parameters Manually

Manual modification of Hard Model parameters becomes reasonable when automatic parameter adjustment does not work as expected. Then, minor manual modifications could remedy these modeling problems. However, manual adjustments should always be followed by automatic parameter fitting to further improve the model.

Changing Parameter Values

The following parameter values can be modified manually using the Model Tree Panel:

- all baseline parameters
- peak parameters of the editable component

The following parameters cannot be modified manually:

- component parameters (component shift and component weight)
- peak parameters of other components than the editable component

Select the Hard Model item in the Model Tree Panel or its graphical representation in the Plot Panel to display the element's parameters in the Properties Panel. Use the table in the Properties Panel to change parameter values.

Fixing Parameters

All model parameters but component weights can be fixed, which means that parameter values are not allowed to get changed during model fitting. Still, parameters can get changed manually.

Select the model item in the Model Tree Panel or its graphical representation in the Plot Panel to display the element's parameters in the Properties Panel. Use the check boxes in the Properties Panel to fix or free parameter values. Baseline parameters and peak parameters can also be fixed all at once from the element's context menu.

> Important note: The position of Hard Model Peaks is influenced by two parameters: the peak position parameter and the component shift parameter. While the former is individual for each peak, the latter is the same for all peaks of a component. Fix both parameters if you do not want Hard Model Peaks to get shifted.

Fixing parameters is useful for reducing model complexity (because less parameters need to be adjusted during model fitting), but at the same time model flexibility is reduced too, because less peak variations in the sample can be explained by the model.

Adding Peaks

> Context menu: Plot Panel > Add Peak (Hard Model)

To add a Hard Model Peak manually, right-click at the desired peak position in the Plot Panel and select **Add Peak (Hard Model)** from the context menu. The new Hard Model Peak has its position and maximum at the clicked point and gets suggested values for the other peak parameters.

Note: New peaks will always be added to the editable component.

Removing Peaks

Menu bar:	Edit Model > Hard Model > Remove Selected Peaks
Context menu:	Model Tree > Hard Model Peak Item > Remove
Context menu:	Plot Panel > Hard Model Peak Plot > Remove

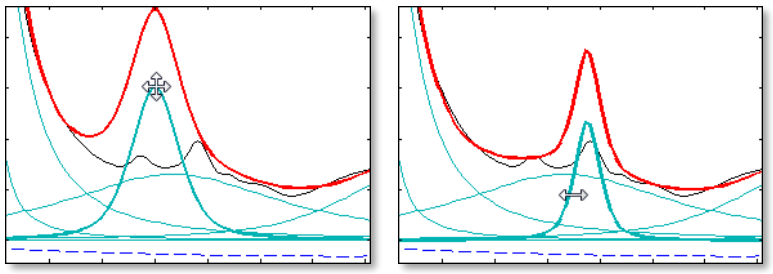
You can remove currently selected Hard Model Peaks. Select a Hard Model Peak in the Model Tree Panel or its graphical representing in the Plot Panel first. In the Plot Panel you could even select multiple peaks while the SHIFT key is pressed.

Only peaks of the editable component can be removed.

Modifying Peaks Interactively

Peaks models can be modified interactively by using the mouse:

- Height and position: Grab the top of an editable peak plot and move the mouse up / down to change the height and move it to the right / left to change the position
- Width: Grab one side of an editable peak plot and move the mouse to the right / left



Caution: You should always respect specified constraints for the peak width parameter when modifying peaks manually. Otherwise, model fitting might not work as expected or might not work at all.

Grouping Peaks

Context menu:	Plot Panel > Peak Plot > Peak Grouping > Group / Ungroup

Grouped peaks behave like a single new peak with new shape. Select two or more peak plots in the Plot Panel (left-click on the plots while the SHIFT key is pressed) and then right-click on one of the plots to open the context menu. From the context menu you could either add all selected peaks to a new group or release peaks from the group. When clicking on a grouped peak in the Plot Panel, the whole group is selected. When clicking on a grouped peak in the Model Tree Panel, only the clicked peak is selected.

Because of the following impacts, peak grouping is relevant for component fitting only:

- The intensity (peak area) of grouped peaks is kept constant as a sum, instead of for each peak individually (see also: Fitting Options).
- If a parameter (e.g., position) of any peak is considered for automatic adjustment, the same kind of parameter will be fitted for all peaks in the group.

Peak grouping is particularly useful to model asymmetric measured peaks by multiple symmetric Hard Model Peaks.

> Caution: Peak grouping should only be used for fine tuning the model.

Switching Baseline Polynomial between Linear and Quadratic

Context menu:	Model Tree > Hard Model Baseline Item > Quadratic Baseline
Context menu:	Plot Panel > Hard Model Baseline Plot > Quadratic Baseline

The Hard Model Baseline can be a linear or quadratic polynomial. The linear baseline has two parameters (offset and slope), the quadratic baseline has three parameters (offset, slope, and quadratic factor).

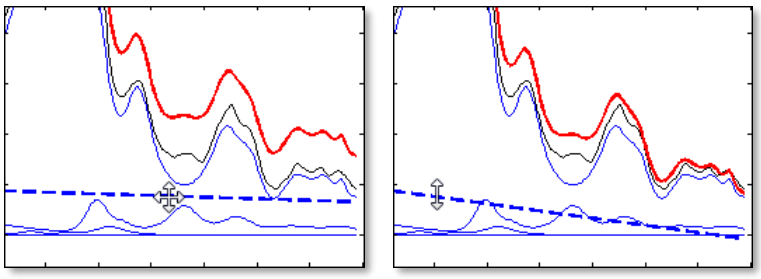
The Hard Model Baseline should be as simple as possible because it is partly redundant to baseline corrections specified in the Pretreatment Model.

> Consider using pretreatments such as range selection and baseline correction to remove background signal, before switching to a quadratic Hard Model Baseline.

Modifying Baseline Interactively

If the Hard Model Baseline is displayed as a separate plot in the Plot Panel (see preferences), it can be modified interactively by using the mouse. In case of a linear function:

- Offset: Grab the center of the baseline plot and move the mouse up / down
- Slope: Grab the left or right fifth of the baseline plot and move the mouse up / down



In case of a quadratic function, baseline parameters are determined by means of three points the baseline goes through. You can adjust the baseline parameters by moving these three points:

- Center point: Grab the center of the baseline plot and move the mouse in any direction
- Leftmost point, rightmost point: Grab the left or right fifth of the baseline plot and move the mouse up / down

3.7.4.12 Adjust Parameters Automatically

Toolbar:	
Menu bar:	Edit Model > Hard Model > Adjust Editable Peaks
Toolbar:	
Menu bar:	Edit Model > Hard Model > Adjust Components > ...

The model's parameter can be adjusted automatically such that the model fits a certain measured spectrum. Model fitting is a crucial step because the Hard Model is intended to represent a mixture spectrum well. A good fit will provide good initial parameter values for subsequent analyses.

There are two kinds of model fitting: peak fitting and component fitting. They differ in parameter constraints being applied and in the set of parameters being adjusted.

Peak Fitting

Peak fitting is suited for creating new Hard Models from the scratch. It is an unconstrained fit (except for bounds on peak width and shape parameters) of editable peaks and therefore it is qualified for making major parameter adjustments, e.g., when adding or removing peaks.

In detail, peak fitting covers:

- adjustment of all parameters of all editable peaks
- adjustment of baseline parameters
- adjustment of component weights

Component Fitting

Component fitting is suited for fine tuning parameters of an existing Hard Model. It is a fit of component weights, but other parameters can be adjusted too according to the chosen parameter set. These additional parameters are fitted with respect to tight constraints. Peak parameters can only vary with respect to constant peak intensities (peak areas). Because of these constraints, component fitting is only qualified for moderate parameter adjustments.

> Note: Component fitting is also performed during some analyses, but while the analysis never changes the Hard Model, during modeling the Hard Model is changed such that adjusted parameter values become new initial values.

Adjusting model parameters by means of component fitting is often not necessary, though in some cases it can be reasonable to get better initial parameter values.

Repeated Model Fitting

When conducting peak fitting or component fitting repeatedly it is likely you will see the fit improving slightly each time. There are several reasons for this, e.g.:

- Stopping criteria for model fitting are measured relative to the starting point. The starting point of each new fit is the previous fit.
- Relative parameter bounds might be reached during one fit. Each new fit has new bounds.

Caution: Repeated component fitting might significantly deform peaks. This could even result in poorer initial parameter values.

3.7.4.13 Settings for Hard Model Fitting

Hard Model fitting is affected by several settings explained in this section.

Peak Fitting

`Default Peak Type`	The default peak function used when adding new peaks to the Hard Model.
	`Pseudo-Voigt`. The Pseudo-Voigt function is a linear combination of Gaussian and Lorentzian functions: $P = \alpha\left[\beta \cdot \exp\left(-\ln(2)\frac{(x-\delta)^2}{\gamma^2}\right) + (1-\beta)\frac{\gamma^2}{(x-\delta)^2+\gamma^2}\right]$ α = peak maximum at the peak's center position β = Gaussian-Lorentzian-ratio between 0 and 1 γ = half width at half maximum (HWHM) δ = center position x = independent variable The area under the peak curve is: $A = \alpha \cdot \gamma\left[\frac{\beta}{\sqrt{\ln(2)/\pi}} + (1-\beta)\pi\right]$
`Auto-Fit Mode`	The mode for adding and fitting new peak functions.
	`Regular (Sequential)`. Peak functions are added and fitted one by one. The next peak function will be added at the position of the largest positive difference between model and signal. This method is slow because all peaks are fitted every time a new peak is added, but sometimes this leads to a better accuracy of the final fit.
	`Fast (Simultaneous)`. Peak functions are added and fitted in groups. Peak positions are determined by means of a peak search. This method is fast and often leads to more physically reasonable results.
`Weighted Auto-Fit`	The option for dealing with noise and peaks of different orders of magnitude when adding and fitting peak functions.

	`Enabled`. Residuals between model and sample are weighted by the absolute sample intensity to consider that noise typically scales with signal intensity, i.e., the noise of a large peak might even be larger than small residual peaks. This way, "noisy peaks" are suppressed, and the next Hard Model Peak is more likely to be added at the position of a real peak.
	`Disabled`. The next peak function is added at the position of the largest positive difference between model and sample.

Absolute Parameter Constraints
Absolute parameter constraints limit values of Hard Model parameters when being adjusted automatically during model fitting. However, parameter constraints can easily be violated by manually setting parameter values outside the constrained range or by tightening constraints such that previous model parameters are then out of bounds. Make sure to not accidentally violate parameter constraints manually.

> Caution: Model fitting may not work correctly for Hard Models with violated parameter constraints.

`HWHM`	Absolute lower and upper bounds for the HWHM (half width at half maximum) parameter.
`Gaussian Part`	Absolute lower and upper bounds for the peak's Gaussian part parameter.

Component Fitting

Component fitting, in general, refers to the adjustment of Hard Model Components to fit a spectrum. Options in this section affect how component fits are performed. However, options are ignored in the following special cases where component fitting is also performed:

- HMFA: here, only weights and baseline parameters are fitted
- Automatic parameter adjustments during hard modeling: here, component fitting is controlled by a separate choice of parameters (see Adjust Components)

`Fitting Mode`	The fitting mode controls the extent of model flexibility, i.e., groups of free model parameters for component fitting. Component fitting modes are named after the main cause for peak variations, namely the extent of molecular interactions among chemical components in a mixture.

	`Minimal Interaction`. Only component weights (W) and baseline (B) parameters are adjusted. This is a linear fit and thus very fast. If the `Component Shift` option is enabled (see below), the fit becomes nonlinear.
	`Medium Interaction`. WB parameters and individual peak positions are adjusted. The actual number of individual peaks being shifted is controlled by the `No. of Considered Peaks` setting (see below).
	`High Interaction`. WB parameters and all peak parameters are adjusted. The actual number of individual peaks being shifted and deformed is controlled by the `No. of Considered Peaks` setting (see below).
	`Maximal Interaction`. All model parameters are adjusted simultaneously. This fit is very time-consuming and can only be recommended for very small models, e.g., if each component only has 1 peak. In that special case the fit may even be faster and result in a smaller fitting error than other modes.
`Component Shift`	This setting can be combined with `Fitting Mode` to enable or disable component shifts. You may use this option to correct for component-wise misalignments. However, consider using the Alignment option of the Pretreatment Model instead if possible.
	`No`. Disabled
	`Yes`. Components get shifted independently of each other as a first step of component fitting. When enabled, the Properties Panel (of the Hard Model item) displays an extra table column to enable or disable shift parameters on a component basis.
`No. of Considered Peaks`	This setting only takes effect if component fitting modes `medium interaction` or `high interaction` are selected. In both cases, the number of adjusted peaks is limited by this setting. The fitting algorithm only considers the most important peaks, i.e., peaks which have the largest influence on improving the fit. Increasing the number of considered peaks increases computational time but does not necessarily increase the goodness of the fit because insignificant peaks might get fitted too. As a rule of thumb, the number of considered peaks should be as high as the number the significant/large peaks in the model.

`Component Weight Threshold`	Hard Model Components with a component weight below the threshold will not be adjusted during component fitting to prevent tiny peaks from getting shifted around and fit noise. The threshold value applies if one would scale the model to a maximum y-value of 1. The threshold value could then be interpreted as a fraction of 1.

Relative Parameter Constraints
Relative parameter constraints define how much a parameter can vary relative to its starting value. Absolute parameter constraints (see above) will still be honored though.

`Component Shift`	Relative bounds (in parameter units) for the component shift parameter. This option is hidden if `Component Shift` (see above) is set to `No`.
`Position`	Relative bounds (in parameter units) for the peak position parameter.
`Max`	Relative bounds (in percent) for the peak maximum parameter.
`HWHM`	Relative bounds (in percent) for the peak HWHM parameter.
`Gaussian Part`	Relative bounds (in parameter units) for the peak's Gaussian part parameter.
`Constant Peak Intensity`	This constraint results from the physical observation, that for a constant concentration, the peak intensity (peak area) is constant even if the peak shape changes, e.g., due to molecular interactions. Therefore, peak shape parameters (maximum, HWHM, and Gaussian Part) are coupled. This should be considered when changing relative constraints for these parameters.

Optimizer Options

Optimizer options are for advanced tuning and should be modified by experienced users only.

Linear Fitting

Linear fitting options apply to component fitting (`Minimal Interaction`) and HMFA. It is recommended not to change the default settings.

`Max. Iterations`	Stopping criterion. Optimization stops after a maximum number of iterations.

`Objective Function Tolerance`	Termination tolerance. Optimization stops only if objective function value drops below the tolerance. The value should be between $1e^{-10}$ and $1e^{-15}$.

Nonlinear Fitting

Nonlinear fitting options apply to peak fitting and component fitting (`Medium Interaction` to `Maximal Interaction`).

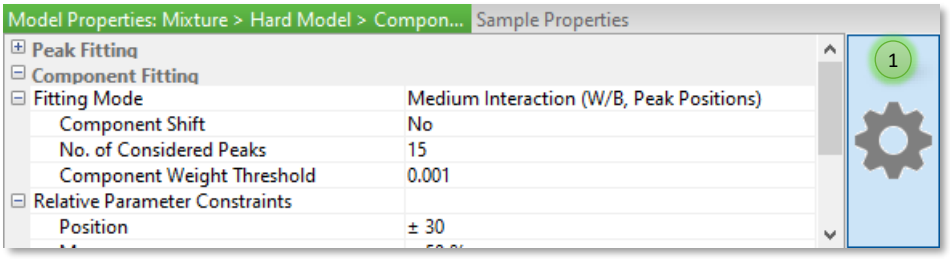
`Max. Iterations`	Stopping criterion. Optimization stops after a maximum number of iterations.
`Objective Function Tolerance`	Termination tolerance. Optimization stops only if objective function value drops below the tolerance. The value should be around $1e^{-6}$.
`Parameter Tolerance`	Termination tolerance. Optimization stops only if progress in improving parameters drops below tolerance. The value should be around $1e^{-6}$.
`Constrained Fitting Algorithm`	This option only applies to constrained optimization problems, i.e., component fitting with `High Interaction` or `Maximal Interaction`.
	`Active-set`. Moderate progress during all iterations. This algorithm typically stops due to small progress. Default termination tolerances should be used.
	`SQP`. Thorough optimization. Good progress at the beginning, steady progress at the end. This algorithm typically stops when the maximum number of iterations is reached. Therefore, the maximum number of iterations should be chosen carefully.
`Constraint Violation Tolerance`	Termination tolerance. Optimization stops only if constraints are violated by less than the tolerance. The value should be around $1e^{-2}$. This option only applies to constrained optimization problems, i.e., component fitting with `High Interaction` or `Maximal Interaction`.

Modification

Properties Panel: Click Model Tree > Hard Model Item > Left-click toggle button

Hard Model settings can be modified by using the Model Properties Panel. Select the Hard Model item or any of its sub-items in the Model Tree Panel and then left-click the toggle button in the

Model Properties Panel. The button toggles between Hard Model parameters and Hard Model settings.



1) Toggle between Hard Model parameters view and Hard Model settings view

Reset

Context menu:	Click Model Tree > Hard Model Item > Right-click toggle button

Hard Model settings can be reset to preferences defined in the active session profile. Right-click the toggle button and choose Reset from the context menu.

3.7.5 Calibration Model

The Calibration Model is a sub-model that is a functional relationship between values calculated from sample spectra (e.g., component weights) and numerical features (e.g., concentrations). The functional relationship is established by regression.

Calibration Models can be utilized for Prediction.

3.7.5.1 New Calibration Model

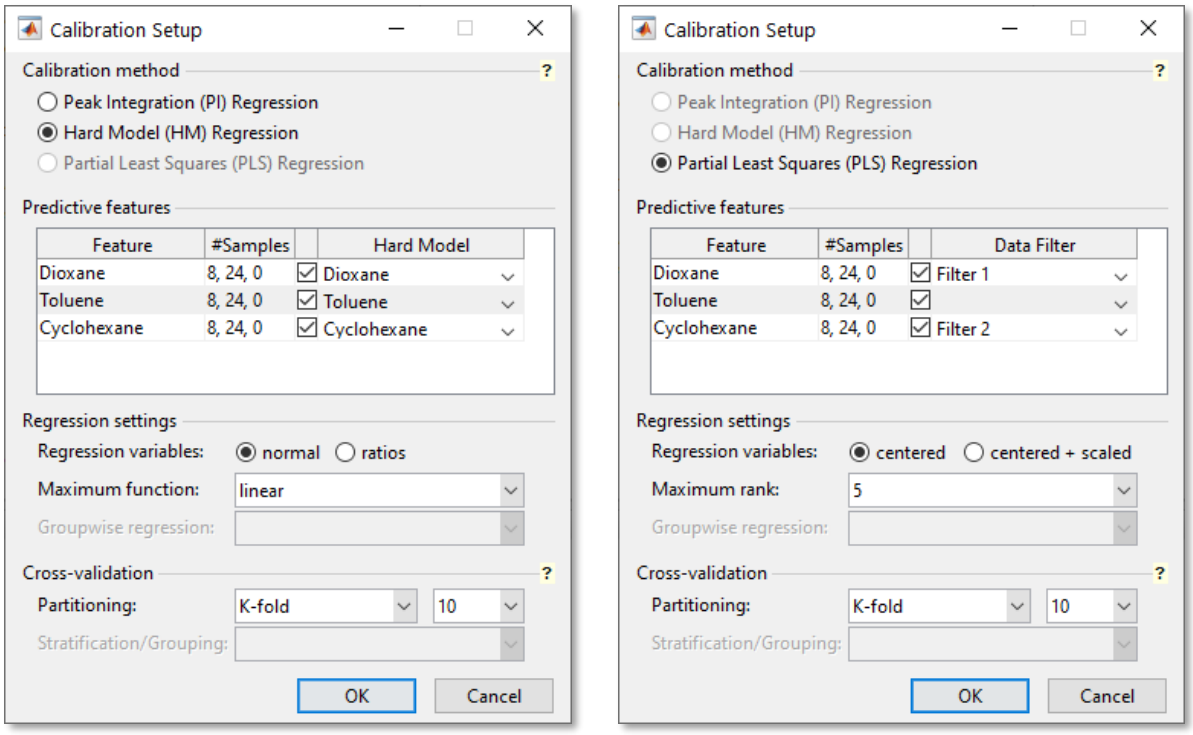
Toolbar	
Menu bar:	Edit Model > Calibration Model > New...
Context menu:	Model Tree > Calibration Model Item > New...

Creates a new Calibration Model and adds it to the active model, replacing a previous Calibration Model if any.

Calibration is performed with selected samples except for those with `Quality` set to `bad`. Samples with `Usage` set to `train` are used for training the Calibration Model. Training samples must provide at least one numerical feature. Samples with `Usage` set to `test` are used for validating the Calibration Model. Samples with `Usage` set to `ignore` have no effect on calibration or validation but are still included in reports.

Calibration begins with a setup dialog. Results are then displayed in a Report Window where you can evaluate the alternative Calibration Models. Finally, you must choose and accept one alternative.

Calibration Setup



Calibration Setup Dialog for univariate (left) and multivariate calibration (right)

`Calibration Method`	The algorithm to be used for calibration. Depending on your choice, the Calibration Setup Dialog changes its appearance to provide proper controls for each method. The following options are available:
	`Peak Integration (PI) Regression.` Univariate regression of feature values on Integration Model Component areas; requires an Integration Model.
	`Hard Modeling (HM) Regression.` Univariate regression of feature values on Hard Model Component weights; requires a Hard Model.
	`Partial Least Squares (PLS) Regression.` Multivariate regression of feature values on spectral intensities. PEAXACT creates separate regressions for each feature (also known as PLS-1) using the SIMPLS algorithm.

`Predictive Features`	The table shows a list of available numerical features and for each the number of available samples with `Usage` = `train`, `test`, and `ignore`. Use the checkboxes to activate/deactivate features for calibration. For `PI`, each active feature must be linked with an Integration Model Component in order to provide a connection between features and component areas. For `HM`, each active feature must be linked with a Hard Model Component in order to provide a connection between features and component weights. For `PLS`, an active feature can optionally be linked with a Data Filter in order to calibrate separate features with separate regions of the spectrum. It is possible to link the same Data Filter to multiple features. If no Data Filter is assigned, the whole spectrum is used.
Regression Settings	
`Regression variables`	A method-dependent modifier that specifies how regression variables should be treated. The following options are available:
	`normal`. Available for univariate regression (PI, HM); regression of the Calibration Model is performed separately for each feature.
	`ratios`. Available for univariate regression (PI, HM) if the sum of active feature values is the same constant for all sample; regression of the Calibration Model is done for pairwise ratios of features and by incorporating the closure constant.
	`centered`. Available for PLS regression; each data point of the spectrum is centered at the mean across all training samples.
	`centered + scaled`. Available for PLS regression; data points are centered, followed by division of each data point by the standard deviation across all training samples.
`Maximum function`	Available for univariate regression (PI, HM); The maximum polynomial degree of the regression function to establish the functional relationship between component areas / weights and numerical features. A separate model will be calibrated for each function from `simple` (= linear function without intercept term) up to the selected maximum.

`Maximum rank`	Available for PLS regression; The maximum number of latent factors used to explain the variance of the data. A separate model will be calibrated for each rank from 1 up to the selected maximum.
`Groupwise regression`	Available if training samples provide categorical features; A separate model will be calibrated for each class of the chosen categorical feature.

Validation settings

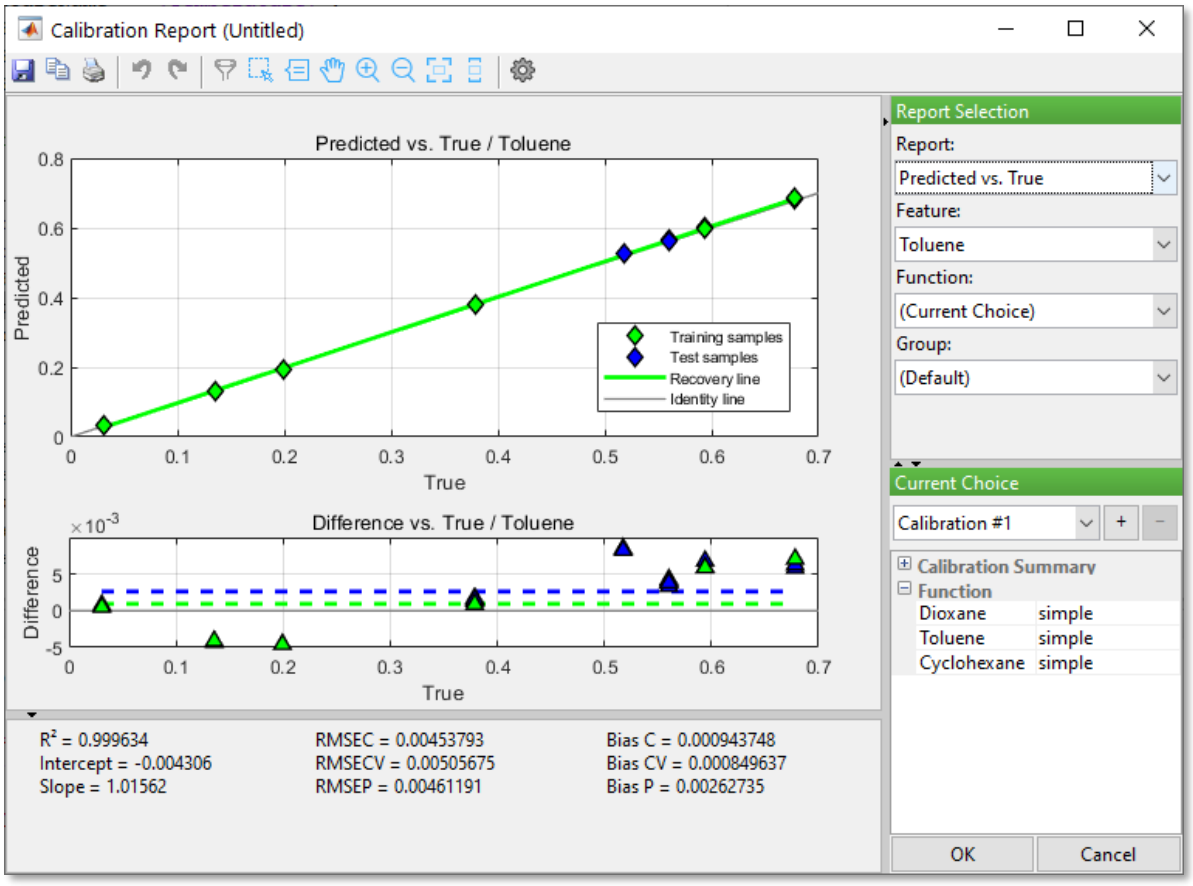
Validation is important to validate the predictive quality of a model. In general, the kind of validation that can be performed depends on the provided data. PEAXACT will always calculate the root mean squared error of calibration (RMSEC) from the training samples. If independent test samples are provided, the root mean squared error of prediction (RMSEP) is calculated as well.

Cross-validation is performed according to the options you choose in the setup dialog. Cross-validation splits the N original training samples into two subsets, one training set to fit the Calibration Model and one test set to compute a validation error, and then re-partitions the subsets until each sample has been used for testing exactly once. The validation errors are averaged over the partitions to give the cross-validation error (RMSECV).

`Partitioning`	The kind of partitioning to be used for cross-validation:
	`None`. Cross-validation is disabled (not recommended).
	`Leave-1-out`. Creates N partitions by leaving out 1 sample for testing each time. Use for small N only!
	`K-fold`. Creates k partitions by leaving out N/k samples each time. k=10 is a widely used standard. You can optionally choose a categorical feature for stratification (see below)
	`Leave-group-out`. Creates partitions by leaving out 1 sample group for testing each time (see below).
	`K-fold groupwise`. Creates k partitions by leaving out N/k sample groups for testing each time (see below).
`Stratification`	For `K-fold` you can optionally choose a categorical feature for stratification. Stratified cross-validation creates subsets which roughly have the same composition of the categorical feature as the whole set of samples.
`Grouping`	For `Leave-group-out` and `K-Fold groupwise` you need to choose a categorical feature for grouping. Samples are treated in groups as defined by a categorical feature. Use this to validate across groups.

Start calibration by clicking the **OK** button.

Calibration Results



Calibration Report Window

Results are displayed in a Report Window. The list of available reports depends on the chosen calibration method.

Available Reports

RMSE vs. Function / Rank

RMSE values are plotted against the regression function (univariate regression) or the rank (PLS). RMSEC is the Root Mean Square Error of Calibration. It is the average deviation between predicted and actual feature values of the training samples.

$$RMSEC = \sqrt{\frac{1}{N}\sum_{i}^{N}\left(x_{predicted,i} - x_{true,i}\right)^2}$$

RMSECV is the Root Mean Square Error of Cross-Validation. It is the average deviation between predicted and actual feature values when doing a cross-validation of training samples. Use this report to determine the regression function / rank with the least error if no independent test samples are available.

$$RMSECV = \sqrt{\frac{1}{N}\sum_{i}^{n}\left(x_{predicted\ CV,i} - x_{true,i}\right)^2}$$

$x_{predicted\ CV,i}$: calculated internally and not displayed in any report.

RMSEP is the Root Mean Square Error of Prediction. It is the average deviation between predicted and actual feature when doing a test-set validation of independent test samples. Use this report to determine the regression function / rank with the least error.

$$RMSEP = \sqrt{\frac{1}{N'}\sum_{i}^{N'}\left(x'_{predicted,i} - x'_{true,i}\right)^2}$$

x': feature values of independent test samples.
N': number of test samples.

R2 vs. Function / Rank

R^2 is the fraction of variance in x which is explained by the Calibration Model. A value of 1 corresponds to 100%. The plot gives an overview of R^2 for different regression functions / ranks.

$$R^2 = 1 - \frac{\sum_i^N\left(x_{predicted,i} - x_{true,i}\right)^2}{\sum_i^N\left(x_{true,i} - \bar{x}_{true}\right)^2}$$

x: feature values (e.g., concentrations) of training samples.
$\bar{x}_{true}$: mean x_{true} of all training samples.
N: number of training samples.

R^2 could be negative if the Calibration Model predicts features worse than a constant function would do. Obviously, such models should be discarded.

Predicted vs. True

Predicted feature values $x_{predicted}$ are plotted against the actual values x_{true} for each sample. Samples are color-coded by their usage (green = training samples, blue = test samples, red = ignored samples). The plot can be used determine the predictive accuracy of the model and to spot feature outliers.

$x_{predicted}$ is calculated from samples Y using the Calibration Model $f(Y, K)$.

$$x_{predicted} = f(Y, K)$$

The structure of function $f(Y, K)$ depends on the calibration method (PI, HM, PLS) and on the regression settings.

A best-fit line though the training points – the recovery function – is added to the chart.

$$x_{recovered} = intercept + slope \cdot x_{true}$$

In case of a perfect calibration, intercept and slope of the recovery function would be zero and one, respectively, i.e., it would match the identity line. The deviation from the identity line can be used as an indicator for the predictive capability of the Calibration Model.

Differences vs. True

Differences between predicted and actual values are plotted for each sample.

$$x_{difference} = x_{predicted} - x_{true}$$

Typically, differences will be distributed around zero. The plot can be used to determine shifts and drifts in the calibration by analyzing the distribution pattern.

A dashed line – the average bias – is added to the chart. The average bias is the mean of the differences.

$$bias = \frac{1}{N}\sum_{i}^{N} x_{difference,i}$$

The average bias is shown for training samples (bias C, green) and test samples (bias P, blue). It can be interpreted as the systematic error of prediction, i.e., predictions are off by this value on average.

Predicted vs. …
Predicted feature values are plotted against a selectable feature. Error bars represent the prediction uncertainty for a 95% level of confidence.

RMS Spectral Residuals vs. True
RMS Spectral Residuals vs. …
The Root Mean Squared Spectral Residuals measure how well the model explains the spectral data. It can be used to spot spectral outliers. The smaller the value the better the model explains the spectral signal.

$$RMS\ Res = \sqrt{\frac{1}{P}\sum_{i}^{P}\left(y_{reconstructed,i} - y_{measured,i}\right)^2}$$

y: spectral intensities.
$y_{reconstructed}$: spectral intensities reconstructed by the model. For HM this is the fitted Hard Model; for PLS it is the reconstruction using R PLS loadings. Spectral residuals are not available for PI models.
P: number of spectral data points.
R: rank of the PLS model.

Mahalanobis distance vs. True
Mahalanobis distance vs. RMS Spectral Residuals
Mahalanobis distance vs. …
The Mahalanobis Distance tells how similar a sample is to the set of training samples and can be used to spot spectral outliers. It is a measure of the multivariate distance from the centroid comprised of the PLS scores of all training samples. The Mahalanobis distance is not available for HM and PI models.

$$MD_i = \sqrt{s_i \cdot (S^T \cdot S)^{-1} \cdot s_i^T \cdot (R-1)}$$

s_i: row vector of R PLS scores of spectrum i for which the MD should be calculated.
S: is the N-by-R matrix of row-wise PLS scores of all training samples.
R: PLS rank.
N: number of training samples.
Superscript T denotes the transposed matrix.
Superscript -1 denotes the inverse matrix.

Calibration curve
The calibration curve is the actual regression function of the Calibration Model. It can only be displayed for univariate calibration (HM and PI).

$$x_i = Y_i \cdot K$$

x: features of training samples.
Y_i: design matrix of component weights (HM) or peak areas (PI) of sample i.
K: vector of regression coefficients (calibration constants).
Note that the regression function is linear in K, but could be nonlinear in component weights or peak areas depending on how the design matrix is built. For instance:

$$x_i = [\omega_i^0 \quad \omega_i^1 \quad \omega_i^2] \cdot [k_0 \quad k_1 \quad k_2]^T$$

would be quadratic in component weights ω.

PEAXACT uses inverse calibration (regression of x on Y) to calculate K. It has been shown that inverse calibration yields more precise predictions of unknowns than classical calibration [Tellinghuisen2000].

Variable Importance in Projection (VIP)
Variable Importance in Projection (VIP) scores estimate the importance of each spectral data point (variable), in the projection used in a PLS model. A data point with a VIP Score close to or greater than 1 (one) can be considered important. Use the plot to select spectral regions of importance by means of a Data Filter. Note that VIP scores are calculated before applying Data Filters which makes the plot suitable for interactively changing Data Filters.

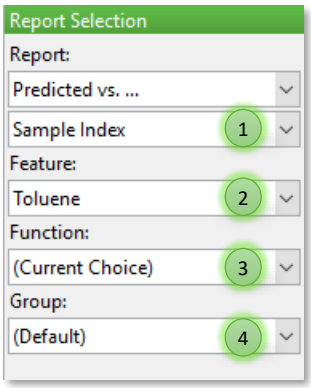
PLS Loadings
PLS loadings allow you to examine how PLS "sees" the data; that is, how it models the original sample spectra by a linear combination of loadings. Typically, at higher ranks, loadings look more and more noisy. As the rank increases, more of the noise in the system is being modeled. Use this report to determine the maximum rank which does not model noise.

$$y_{reconstructed,i} = s_i \cdot L^T$$

$y_{reconstructed,i}$: reconstruction of spectrum i.
s_i: row vector of R PLS scores of spectrum i.
L: P-by-R matrix of column-wise loadings. Loadings are calculated from training samples using the SIMPLS algorithm.
R: rank of the PLS model.
P: number of data points.

PLS Regression Coefficients
PLS regression coefficients show how each spectral data point is related to a calibrated feature across all PLS factors, i.e., from factor 1 to rank R. As the rank increases, more of the noise in the system is being modeled. Use this report to determine the maximum rank which does not model noise.

Report Customization



X-Axis

For several reports you can change the x-axis to any provided sample feature (1). See Data Table Editor for how to add features to samples.

Component Selection

Use the drop-down list (2) to display results for individual Calibration Model Components (features).

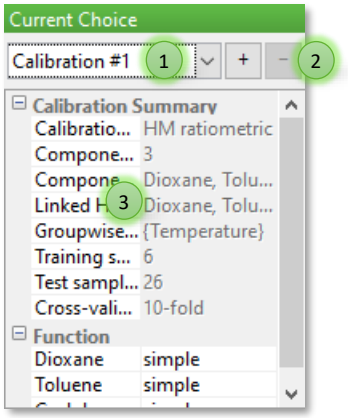
Function / Rank

Use the drop-down list (3) to display results for individual regression functions / ranks. Select **(Current Choice)** to use the function / rank that is currently selected in the Current Choice Panel (see below).

Group

In case of groupwise calibration, use the drop-down list (4) to display results for individual groups of the categorical feature. Select **(Default)** to display the combined results of all groups.

Creating Calibration Model Alternatives



The Calibration Report Window displays results of the selected Calibration Model alternative. Calibration Model alternatives represent separate Calibration Models which can be created and compared within the Report Window.

1) Use the drop-down list to switch between different Calibration Model alternatives.
2) Click **[+]** to add a new alternative. Doing so will display the Calibration Setup Dialog again so that you can try out and compare different calibration settings. The new alternative will be added to the list (1). Click **[-]** to remove the currently selected alternative from the list.
3) The table displays a summary of the currently selected Calibration Model.

Modifying Calibration Model Alternatives

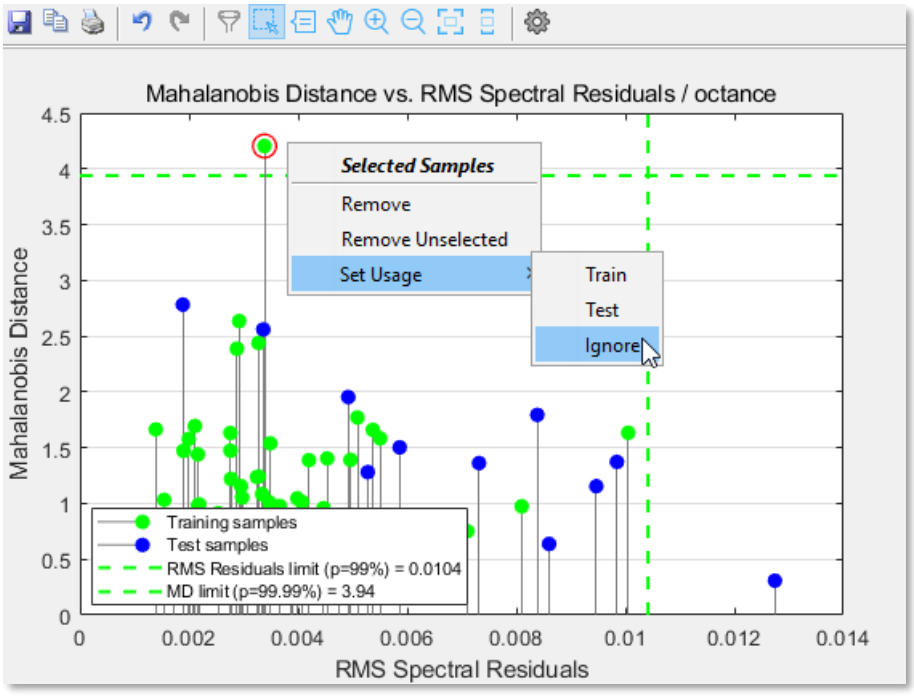
The currently selected Calibration Model alternative can be modified step-by-step to further improve it. The following modifications are possible:

- Changing the sample `Usage`, e.g., switch between `train` and `test`, or `ignore` samples from calibration.
- Changing Data Filters (available for PLS only).

Each modification step automatically triggers a re-calibration and updates the selected Calibration Model, i.e., a modification does not create a new alternative but changes the selected alternative. However, you can undo/redo all modification steps using the Undo/Redo tools from the toolbar.

Changing the Sample Usage

Enable the Selection Tool in the toolbar and select individual samples in graphical reports. Right-click and select the new `Usage` from the context menu to trigger a re-calculation of the Calibration Model with the new `Usage`.



Changing Data Filters

In the top-right pane of the Report Window, select the feature for which you want to edit the Data Filter and switch to any of the following reports:

- Variable Importance in Projection (VIP), or

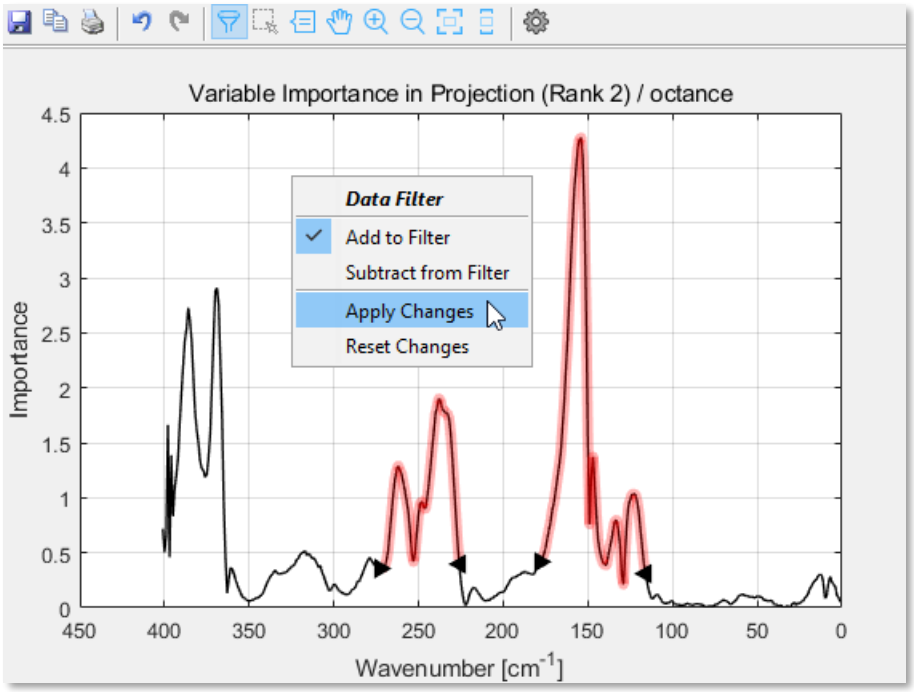
- PLS Loadings, or
- PLS Regression Coefficients.

Enable the Data Filter Tool in the toolbar.

> Note: The Data Filter Tool is only available if a Data Filter was linked to the selected feature during calibration setup.

When the Data Filter Tool is enabled, the Data Filter is displayed in the graph and can be modified with the mouse. When a Data Filter has unsaved modifications, it is displayed in red. Otherwise it is displayed in black. Right-click and select `Apply Changes` from the context menu to trigger a re-calculation of the Calibration Model with the changed Data Filter. Select `Reset Changes` if you want to revert all changes.

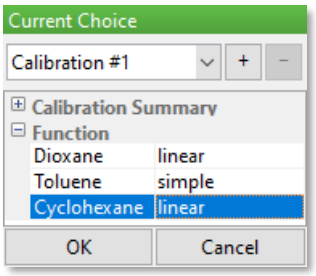
If a Data Filter is assigned to more than one feature, you should check your modifications with all features before accepting it. As a precaution, a warning is shown when you attempt to modify a Data Filter that is assigned to multiple features.



Undo / Redo
Select the Undo Tool or the Redo Tool in the toolbar to navigate through the modification steps of the selected Calibration Model alternative. Each Undo/Redo action will trigger a re-calculation of the Calibration Model to restore the model.

Accepting a Calibration Model Alternative

To finalize calibration, you must decide on a specific Calibration Model alternative and must select a specific regression function / rank for each calibrated feature. Make your choice in the bottom-left pane of the Report Window.



By clicking the **OK** button of the Report Window, your choice is accepted, and the Calibration Model is added to the active model. Any changes to the sample `Usage` or to Data Filters are copied to the main window. Unused Calibration Model alternatives will be discarded.

3.7.5.2 Remove Calibration Model

Menu bar:	Edit Model > Calibration Model > Remove
Context menu:	Model Tree > Calibration Model Item > Remove

Removes the Calibration Model from the active model. Removing the Calibration Model also removes dependent elements such as Custom Results. Note that you cannot remove single Calibration Model Components but only the whole model.

3.7.5.3 View

Menu bar:	Edit Model > Calibration Model > View
Context menu:	Model Tree > Calibration Model Item > View

You can view the results of current calibration again in the Calibration Report Window, where all standard reports are available.

Since the calibration report is opened in "View Mode", options that would change the Calibration Model are disabled.

3.7.5.4 Rename Component

Menu bar:	Edit Model > Calibration Model > Rename Component...
Context menu:	Model Tree > Calibration Model Component Item > Rename
Properties Panel:	Click Model Tree > Calibration Model Item

Renames the selected Calibration Model Component. A component can have any name if it is unique within the Calibration Model.

This operation applies to after a Calibration Model has been created. To change feature names prior to calibration, use the Data Table Editor.

3.7.6 Classification Model

The Classification Model is a sub-model that is a functional relationship between sample spectra and the levels (categories) of a categorical feature. The functional relationship is established by classification.

Classification Models can be utilized for Identification.

3.7.6.1 New Classification Model

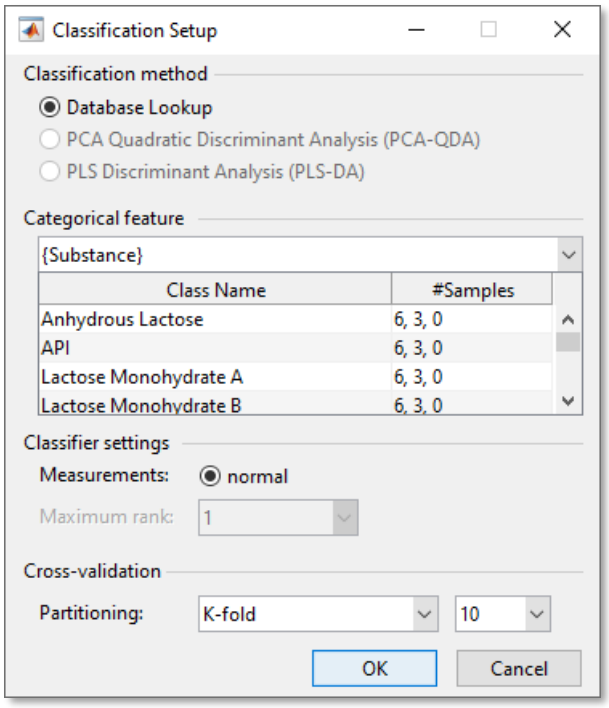
Toolbar	
Menu bar:	Edit Model > Classification Model > New...
Context menu:	Model Tree > Classification Model Item > New...

Creates a new Classification Model and adds it to the active model, replacing a previous Classification Model if any.

Classification is performed with selected samples except for those with `Quality` set to `bad`. Samples with `Usage` set to `train` are used for training the Classification Model. Training samples must provide a least one categorical feature. Samples with `Usage` set to `test` are used for validating the Classification Model. Samples with `Usage` set to `ignore` have no effect on classification or validation but are still included in reports.

Classification begins with a setup dialog. Results are then displayed in a Report Window where you can evaluate alternative Classification Models. Finally, you must choose and accept one alternative.

Classification Setup



`Calibration Method`	The algorithm to be used for classification. Depending on your choice, the Classification Setup Dialog changes its appearance to provide proper controls for each method. The following options are available:
	`Database Lookup`. Spectra of training samples are used as a database against which new samples are later matched. The matching (or lookup) is done according to smallest Pearson distance (largest Pearson correlation) and returns the class name of the most similar database sample.
	`PCA Quadratic Discriminant Analysis (PCA-QDA)`. Added soon.
	`PLS Discriminant Analysis (PLS-DA)`. Added soon.
`Categorical Feature`	Use the drop-down list to select a categorical feature for which the model should be trained. The table shows available classes of the selected feature and the number of available samples with `Usage` = `train`, `test`, and `ignore`. For method `Database Lookup`, a special feature `Sample Name` is available which treats each sample as a separate class. For this to work, all samples must have `Usage = train`.

Classifier Settings

`Measurements`	A method-dependent modifier that specifies how spectra should be treated. The following options are available:
	`normal`. Available for `Database Lookup`; spectra are not modified.
	`centered`. Available for PC-based methods; each data point of the spectrum is centered at the mean of that data point across all training samples.
	`centered + scaled`. Available for PC-based methods; data points are centered, followed by division of each data point by the standard deviation of that data point.
`Maximum rank`	Available for PC-based methods; The maximum number of principal components used for dimensional reduction of the spectra. A separate model will be trained for each rank from 1 up to the selected maximum.

Validation settings

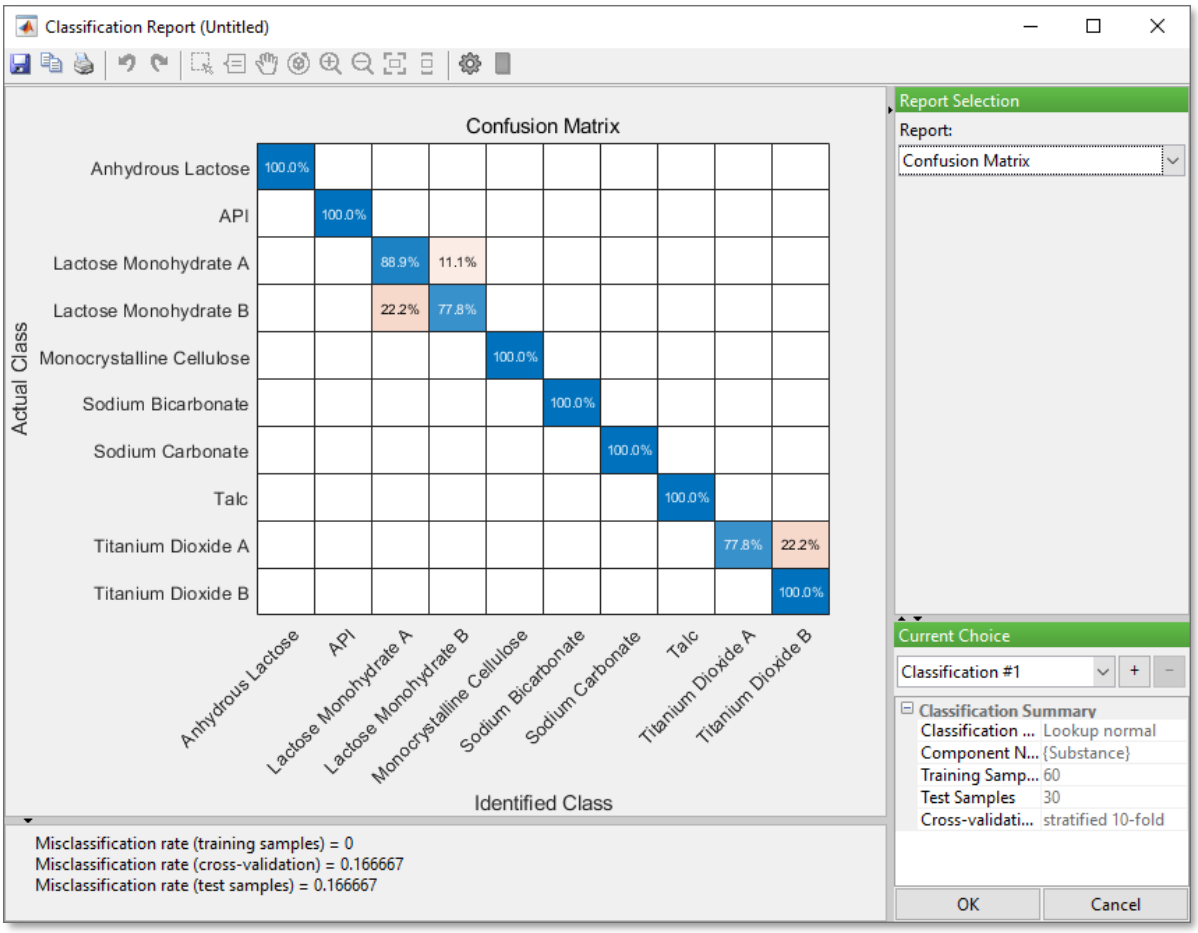
Validation is important to validate the predictive quality of a model. In general, the kind of validation that can be performed depends on the provided data. PEAXACT will always calculate the misclassification rate of training samples. If independent test samples are provided, the misclassification rate of test samples is calculated too.

Cross-validation is performed according to the options you choose during classification setup. Cross-validation splits the N original training samples into two subsets, one training set to train the Classification Model and one test set to compute a validation error, and then re-partitions the subsets until each sample has been used for testing exactly once. The validation errors are averaged over the partitions to give the misclassification rate of cross-validation.

`Partitioning`	The kind of partitioning to be used for cross-validation:
	`None`. Cross-validation is disabled. For `Database Lookup` of feature `Sample Name`, this is the only option. For other methods, this is not recommended.
	`Leave-1-out`. Creates N partitions by leaving out 1 sample for testing each time. Use for small N only!
	`K-fold`. Creates k partitions by leaving out N/k samples each time. k=10 is a widely used standard. K-fold cross-validation is always stratified. Stratified cross-validation creates subsets which roughly have the same composition of the categorical feature as the whole set of samples.

Start classification by clicking the **OK** button.

Classification Results



Classification Report Window

Results are displayed in a Report Window. The list of available reports depends on the chosen classification method.

Available Reports

Misclassification Rate / Error rate

The misclassification rate (also known as error rate) is an overall measure for how often the Classification Model incorrectly identifies the class of a sample. It is the ratio of the number of incorrectly identified samples to the number of all samples. Misclassification rates can also be calculated separately for the set of training samples, for cross-validation, and for the set of test samples.

Confusion Matrix

A graphical visualization of the row-wise percentage of correctly identified classes (main diagonal) and incorrectly identified classes (off-diagonals). E.g., a perfect classification would have 100% values on the main diagonal. Numbers are calculated from the combined set of training and test samples.

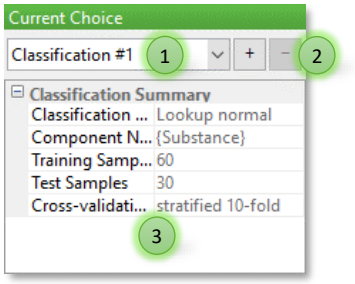
Use the confusion matrix to inspect the performance of the Classification Model on a per-class basis.

Identified Class vs …
Identified class names are plotted against a selectable feature. In addition, samples can be colored by a second feature.

Table: Confusion Matrix
A tabular visualization of the correctly identified class counts (main diagonal) and incorrectly identified class counts (off-diagonals). A row-wise summary of misclassification rates is added to the right of the table. Numbers are calculated from the combined set of training and test samples.

Table: Classification Details
Table of all results per sample.

Creating Classification Model Alternatives



The Classification Report Window displays results of the selected Classification Model alternative. Classification Model alternatives represent separate Classification Models which can be created and compared within the Report Window.

1) Use the drop-down list to switch between different Classification Model alternatives.
2) Click **[+]** to add a new alternative. Doing so will display the Classification Setup Dialog again so that you can try out and compare different classification settings. The new alternative will be added to the list (1). Click **[-]** to remove the currently selected alternative from the list.
3) The table displays a summary of the currently selected Classification Model.

Modifying Classification Model Alternatives

The currently selected Classification Model alternative can be modified step-by-step to further improve it. The following modifications are possible:

- Changing the sample `Usage`, e.g., switch between `train` and `test`, or `ignore` samples from classification.

Each modification step automatically triggers a re-classification and updates the selected Classification Model, i.e., a modification does not create a new alternative but changes the selected alternative. However, you can undo/redo all modification steps using the Undo/Redo tools from the toolbar.

Changing the Sample Usage
Enable the Selection Tool in the toolbar and select individual samples in graphical reports. Right-click and select the new `Usage` from the context menu to trigger a re-calculation of the Classification Model with the new `Usage`.

Undo / Redo
Select the Undo Tool or the Redo Tool in the toolbar to navigate through the modification steps of the selected Classification Model alternative. Each Undo/Redo action will trigger a re-calculation of the Classification Model to restore the model.

Accepting a Classification Alternative

By clicking the **OK** button of the Report Window, the selected Classification Model is added to the active model. Any changes to the sample `Usage` are copied to the main window. Unused Classification Model alternatives will be discarded.

3.7.6.2 Remove Classification Model

Menu bar:	Edit Model > Classification Model > Remove
Context menu:	Model Tree > Classification Model Item > Remove

Removes the whole Classification Model. Removing the Classification Model also removes dependent elements such as Custom Results.

3.7.6.3 View

Menu bar:	Edit Model > Classification Model > View
Context menu:	Model Tree > Classification Model Item > View

You can view the results of the current classification again in the Classification Report Window, where all standard reports are available.

Since the calibration report is opened in "View Mode", options that would change the Classification Model are disabled.

3.7.6.4 Rename Component

Menu bar:	Edit Model > Classification Model > Rename Component...
Context menu:	Model Tree > Classification Model Component Item > Rename
Properties Panel:	Click Model Tree > Classification Model Item

Renames the Classification Model Component.

Note: This operation applies to after a Classification Model has been created. To change feature names prior to classification, use the Data Table Editor.

3.7.7 Custom Model

The Custom Model is a sub-model that contains any number of user-defined custom results. There are two kinds of custom results:

- Results of built-in analyses: Integration, Component Fitting, Prediction, Identification.
- Results calculated from user-defined expressions.

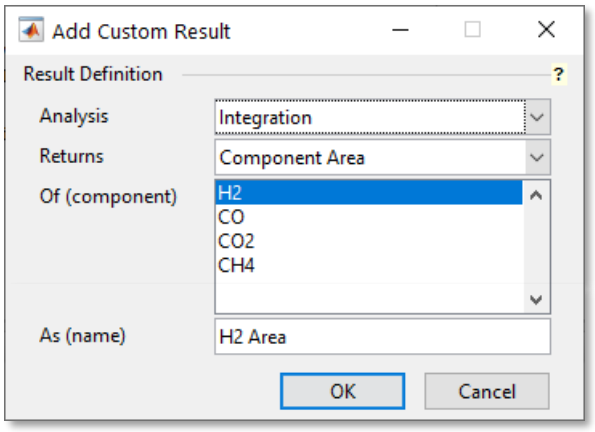
Building a Custom Model typically starts with adding results of built-in analyses which then can be referenced in user-defined expressions.

Custom Models can be utilized for Custom Analyses.

3.7.7.1 Add Result

Toolbar:	
Menu bar:	Edit Model > Custom Results > Add...
Context menu:	Model Tree > Custom Results Item > Add...

Adds a new Custom Result by using the dialog to specify properties of the result.



`Analysis`	The kind of analysis to be performed. This is either one of the built-in analyses (`Integration`, `Component Fitting`, `Prediction`, `Identification`) where you can pick from a list of available result values, or `Custom`, which lets you write custom expressions to calculate new values.
`Returns`	The kind of result value to be returned by the analysis. For `Custom` you need to specify whether your custom expression will return a numeric value or categorical value (text). For built-in analyses you can pick from a list that depends on the kind of analysis.

`Of (component)`	Required for built-in analyses only; A reference to the model component that provides the result value. Each model component has an internal ID to which references are linked. You can safely rename referenced components without breaking the reference, but if you remove or replace a component all references to it will be broken. You need to repair broken references (see Edit Result Definition) or remove them.
`As (name)`	The name of the result to be displayed in reports. Results can get any name if it is unique within the Custom Model.

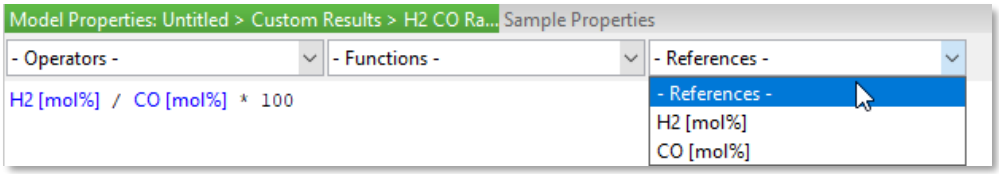
Click **OK** to add the result to the Custom Model. For results with `Analysis = Custom`, continue with writing the custom expression.

3.7.7.2 Write Custom Expressions

Properties Panel: Click Model Tree > Custom Result Item

Custom Results of type `Analysis = Custom` consist of a user-defined custom expression. A custom expression represents the left-hand side of an equation
`result = custom expression`.

Custom expressions can be edited in the Model Properties Panel. Select a Custom Result item in the Model Tree Panel to show the editor.



Use the editor to write a custom expression, including operators, functions, and references to other custom results.

After modifying the custom expression, press the ENTER key to save changes.

Note: The editor turns yellow when an expression has unsaved changes.

Numbers and Text

Custom Results can be configured to return either numerical values or categorical (text) values. Make sure that your expression evaluates to the configured type. You can use conversion functions `NUMBER()` and `TEXT()` to convert between types.

Syntax for numeric literals: `123, 3.1415, .5, 1e03, +27, -0.9, -1.23e-45`
Syntax for text literals: `"ABC", "Level 4", "1.23", ""` (empty text)
Combining numbers and text: `"PI = " + TEXT(3.1415), 100 >= NUMBER("99")`

Syntax Errors and Runtime Errors

When pressing the ENTER key in the custom expression editor, PEAXACT perform basic syntax checks and displays appropriate error messages. Runtime errors on the other hand are harder to detect as they only occur when custom expressions are evaluated. How runtime errors are treated depends on the software environment where the model is executed. E.g., the PEAXACT main window displays an error dialog, while the PEAXACT AppServer throws an exception to be handled by third-party software. Therefore, make sure to test the model adequately, e.g., by performing a Custom Analysis to see whether all results get calculated correctly.

Operators

Arithmetic Operators

`x + y`	For numeric x and y: Add x and y. For categorical x and y: Concatenate text.
`x - y`	Subtract y from x.
`x * y`	Multiply x and y.
`x / y`	Divide x by y.
`x^y`	Raise x to the power of y.

Relational Operators

`x == y`	Returns true (1) if x is equal to y, false (0) otherwise.
`x != y`	Returns true (1) if x is not equal to y, false (0) otherwise.
`x <= y`	Returns true (1) if x is less than or equal to y, false (0) otherwise.
`x >= y`	Returns true (1) if x is greater than or equal to y, false (0) otherwise.
`x < y`	Returns true (1) if x is less than y, false (0) otherwise.
`x > y`	Returns true (1) if x is greater than y, false (0) otherwise.

Logical Operators

`x && y`	Returns true (1) if both x and y evaluate to true, false (0) otherwise.
`x || y`	Returns true (1) if either x or y evaluates to true, false (0) otherwise.

Operator Precedence

You can build expressions that use any combination of arithmetic, relational, and logical operators. Precedence levels determine the order in which expressions are evaluated. Within each precedence level, operators have equal precedence and are evaluated from left to right. The

precedence rules are shown in the list below, ordered from highest precedence level to lowest precedence level:

- Parentheses ()
- Power (^)
- Power with unary minus (^-), unary plus (^+). Although most operators work from left to right, the operators (^-) and (^+) work from second from the right to left. It is recommended that you use parentheses to explicitly specify the intended precedence of statements containing these operator combinations.
- Unary plus (+), unary minus (-)
- Multiplication (*), division (/)
- Addition (+), subtraction (-)
- Less than (<), less than or equal to (<=), greater than (>), greater than or equal to (>=), equal to (==), not equal to (!=)
- Logical AND (&&)
- Logical OR (||)

The default precedence can always be overridden using parentheses.

Functions

Mathematical Functions

`SQRT(x)`	Returns the square root of a number.
`MIN(x, y)`	Returns the smaller of two numbers.
`MAX(x, y)`	Returns the larger of two numbers.
`ROUND(x)`	Returns `x` rounded to the nearest integer.
`ROUND(x, n)`	Returns `x` rounded to `n` significant digits.

Logical Functions

`IF(condition, x, y)`	Returns `x` if `condition` evaluates to true, `y` otherwise. `x` and `y` must either both be numbers, or both be text. `condition` must evaluate to a number, where `0` is considered as false and any other value is considered as true. The `condition` can contain relational and logical operators, e.g.,
	`IF(y == 0 || (x > 40 && x < 60), x, y)`
	`IF(x == "A", "valid", "invalid")`

Conversion Functions

`NUMBER(text)`	Converts `text` into a number.
`TEXT(number)`	Converts `number` into text.

Nested Functions
You can build expressions that use any combination of functions. Functions can be nested, i.e., the input argument of a function can be another function. Within the expression, functions are evaluated from left to right and from inner-most to the outer function.

References

You can build expressions that contain references to other custom results. When the expression gets evaluated, references get replaced by the value of the referenced result.

In the expression editor, position the cursor where you want to insert a reference. Then select the corresponding result from the **References drop-down list**. The name of the referenced result is displayed as blue text block. The text block behaves like regular text, i.e., it can be deleted, selected, copied, and pasted. However, a reference belongs to a specific model, i.e., you cannot copy and paste references between different models.

Broken References
Each custom result has an internal ID number to which references are linked. You can safely rename results without breaking a reference, but if you remove a result all references to it will be broken. Broken references are displayed in the expression editor as blue text block starting with `#Ref` followed by the last known name of the removed result. Broken references must be updated or removed from the expression before custom results can be evaluated.

3.7.7.3 Edit Result Definition

Menu bar:	Edit Model > Custom Results > Edit...
Context menu:	Model Tree > Custom Results Item > Edit...

You can change the definition of a custom result if needed, e.g., modify the kind of analysis, result type, referenced model component, or result name. This is done with the same dialog that was used when adding the result (see Add Result).

Repairing Broken References

Note: The section is about references used in custom results of built-in analyses. For references used in custom expressions, see Write Custom Expressions.

Assume there exists a Custom Result of a built-in analysis (e.g., `Analysis = Prediction)` which is referencing a Calibration Model Component `Cyclohexane`. Now, when the model gets re-calibrated, the Calibration Model gets replaced and the Custom Result refers to a component that does not exist anymore. The reference is broken and must be repaired. You probably want the Custom Result to reference a component of the new Calibration Model instead. In such case, edit the custom result, select the new component from the dialog, and click OK.

3.7.7.4 Rename Result

Menu bar:	Edit Model > Custom Results > Rename
Context menu:	Model Tree > Custom Result Item > Rename
Properties Panel:	Click Model Tree > Custom Results Item

Renames the selected Custom Result. A Custom Results can get any name if it is unique within the Custom Model.

3.7.7.5 Remove Result

Menu bar:	Edit Model > Custom Results > Remove
Context menu:	Model Tree > Custom Result Item > Remove

Removes the selected Custom Result. Removing Custom Results may affect other Custom Results which depend on them.

3.8 Analysis

Data analysis is a process of transforming data such as to highlight and extract useful information that is otherwise hidden in the data.

PEAXACT follows and supports the typical analysis workflow, starting with data-driven analyses to visualize and explore the data, followed by model-based analyses to convert measured data to quantities of interest.

Data-driven analyses can be performed with the Data Inspector. This section is dedicated to the specifics of model-based analyses.

Typical Analysis Workflow

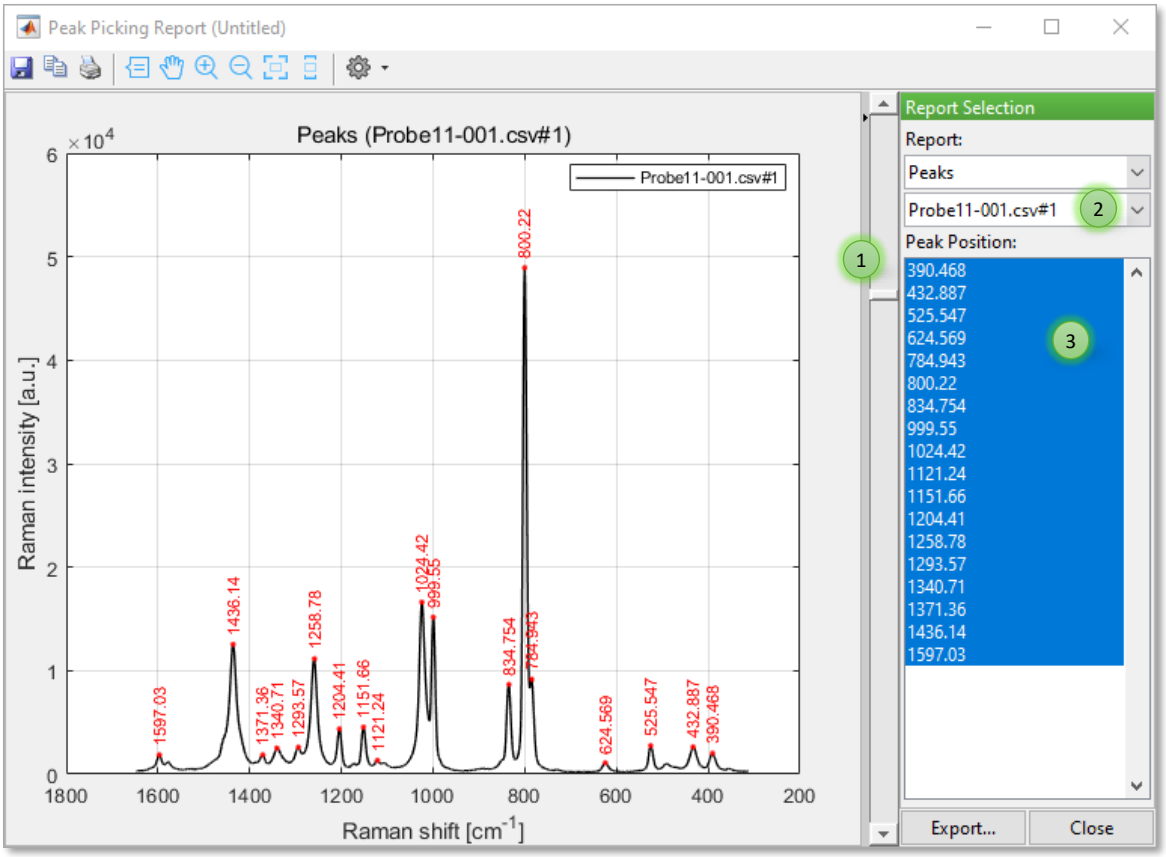
- Select samples In the Samples Panel that you want to analyze. Samples with `Quality` set to `bad` will be ignored.
- Choose an analysis method from the Analysis menu. Method availability depends on the active model. E.g., to perform a prediction, the model must be calibrated. Some analyses do not require a model but may work better / differently if one is provided.
- Some analyses need additional input.
- Wait for the analysis to complete. Processing time depends on the chosen analysis method, on the number of selected samples, and on the performance of your computer.
- Explore results in a Report Window.

3.8.2 Peak Picking

Menu bar:	Analysis > Peak Picking

Finds local maxima (peaks) in the spectrum and displays corresponding x- and y-values. Results are displayed in a Report Window.

Peak picking is performed for the selection in the Samples Panel, not including samples with `Quality = Bad`. A model is not required for this analysis, but if one is active, data pretreatments are applied.



Available Reports

Peaks

Positions of peaks plotted (in red) into chart of selected sample (black)

Report Table

Table with numeric values of peak positions and peak intensities

Report Customization

Peak Detection Limit

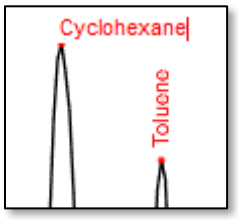
Move the slider (1) up and down to increase and decrease the detection limit of peaks.

Sample Selection

The report shows results for a single sample at a time. Select the visible sample from the drop-down list (2).

Peak Selection
By default, all detected peaks are shown in the graphical and tabular report. Use the list (3) to select and show specific peaks only.

Edit Peak Label
Left-click on the red peak label to start editing. Note that labels will be reset each time you change the peak detection limit, the sample, or the peak selection.



3.8.3 MCR-ALS

Menu bar:	Analysis > MCR-ALS > Component Number Analysis
Menu bar:	Analysis > MCR-ALS > Component Analysis

Multivariate Curve Resolution (MCR) Alternating Least Squares (ALS) intends the recovery of the pure response profiles (spectra, pH profiles, time profiles, elution profiles ...) of the chemical constituents or species of an unresolved mixture when no prior information is available about the nature and composition of these mixtures.

MCR is performed for the selection in the Samples Panel, not including samples with `Quality = Bad`. A model is not required for this analysis, but if one is active, data pretreatments are applied.

The Bilinear Model of MCR

MCR requires the experimental data to be explained reasonably well by a bilinear model using a limited number of components. The MCR bilinear model is usually written down as $D = CS^T$, where D is the spectroscopic data matrix, and S^T and C are the matrices of the pure spectra and the related concentration profiles for each of the compounds (contributions) in the system. C and S^T are the small matrices of the bilinear model that contain profiles of the pure contributions (species, compounds) of the original data matrix and may change chemical meaning depending on the nature of the data

MCR-ALS is an algorithm that solves the MCR basic bilinear model using a constrained Alternating Least Squares algorithm. The constraints used to improve the interpretability of the profiles in C and S^T may respond to chemical properties of these profiles (e.g., non-negativity, unimodality, closure ...) or have a mathematical origin (e.g., local rank and selective windows, trilinear structure ...). The 'art' and expertise in using MCR-ALS stems from the proper selection and application of the constraints that are really fulfilled by the data.

3.8.3.2 Component Number Analysis

Menu bar:	Analysis > MCR-ALS > Component Number Analysis

Estimates the number of unknown mixture constituents by means of different figures of merit. Results are displayed in a Report Window.

Available Reports

Explained Variance
Each component contributes to explaining the variance of the data matrix. The most likely number of components is reached when the next component does not significantly increase the explained variance anymore.

RMS Residuals of PC Reconstruction
A principal component analysis (PCA) is performed and then an assessment is made of how well each number of principal components (PCs) reconstructs the original data matrix by averaging the RMS residuals across all samples. The most likely number is reached when the next component does not significantly reduce the average RMS residuals anymore.

Ratios
The ratios plot supplements the Average-RMS-residuals-plot and the Variances-plot by showing the ratios of two successive RMS-values and variances, respectively. The most likely number of components is indicated by a large ratio.

PCA Scores
PCA scores can be interpreted as abstract component concentration profiles. Assuming the data matrix originates from an experiment with smooth concentration profiles, the most likely number of components is reached when the scores change from a smooth to a noisy profile.

PCA Loadings
PCA loadings can be interpreted as abstract component signal intensities. The most likely number of components is reached when the loadings change from a smooth to a noisy profile.

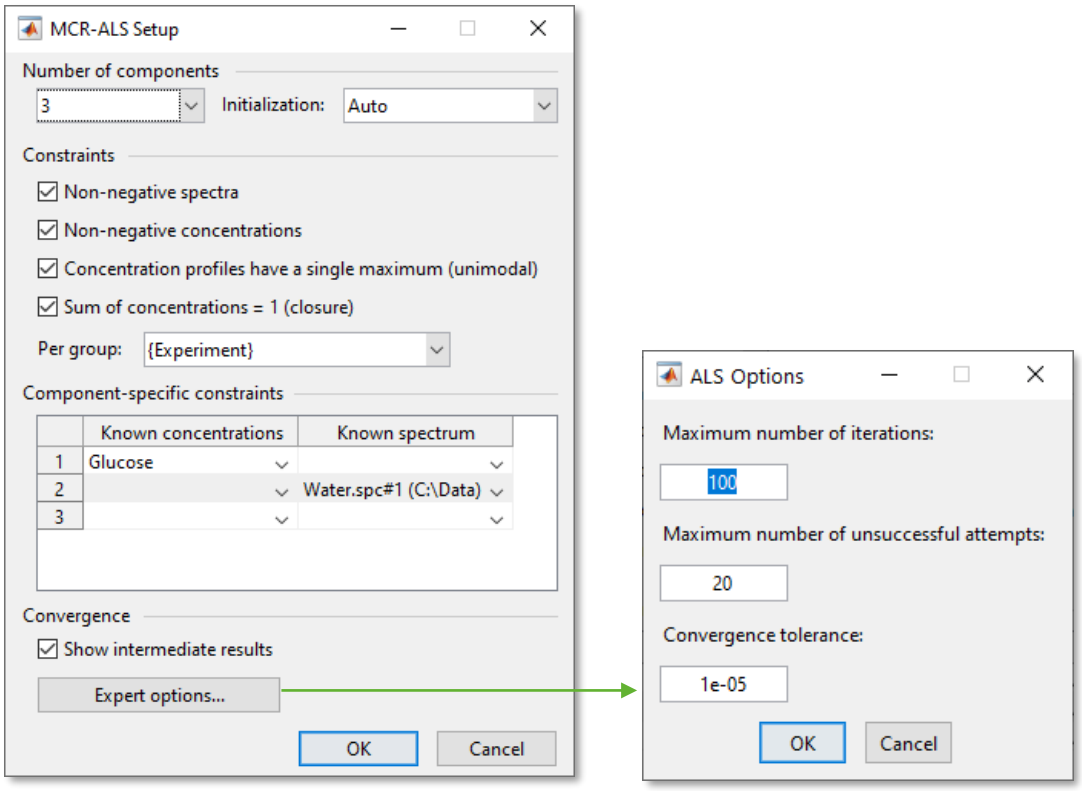
Factor Indicator Function
The factor indicator function reaches a minimum where the correct number of factors/components is expected. However, this only occurs when the error is random and uniform throughout the entire data. [E. R. Malinowski, Analytical Chemistry, Vol. 49 (4), April 1977]. In real cases, the function is typically L-shaped for about the first 10 components and the most likely number of components is indicated by a sharp bend in the curve.

3.8.3.3 Component Analysis

Menu bar:	Analysis > MCR-ALS > Component Analysis

Identifies unknown component spectra and component concentrations from a set of mixture spectra. Results are displayed in a Report Window. Additional input is required for this analysis.

Setup



`Number of components`	The number of components to be identified. Changing the number will adjust the table of component-specific constraints (see below) to the same number of rows.
`Initialization`	The initialization of component spectra or concentrations.
	`Auto`. Uses results from previous iterations if available or option `Purest spectra` otherwise. It is the best option in general.
	`Purest spectra`. Uses least correlated mixture spectra. It is the best option in most cases, particularly when peaks are strongly overlapping.
	`Purest concentrations`. Uses least correlated peak profiles. It is the best option when characteristic peaks exist.

Constraints

Optionally, you can specify constraints to improve the outcome of the analysis

`Non-negative spectra`	Enable this constraint if y-values of pure component spectra are positive. This is usually valid for spectroscopic and chromatographic data. However, it does not hold if you use a Pretreatment Model with derivatives.

`Non-negative concentrations`	Enable this constraint if concentration values are positive. This is usually valid for molar or weight concentrations/fractions.
`Concentration profiles with single maximum (unimodal)`	Enable this unimodality constraint if the shape of concentration profile has a single maximum. This also applies to profiles which are monotonously increasing or decreasing.
`Sum of concentrations = 1 (closure)`	Enable this closure constraint if component concentrations sum up to 1.
`Per group`	Select a categorical feature to apply the unimodality constraint to samples of each group separately. E.g., this allows using samples of multiple experiments, each having concentration profiles with a single maximum.

Component-specific constraints

Optionally, you can specify component-specific constraints. Use the table to specify whatever information you have available about the components that should be identified (see `Number of components`).

`Known concentrations`	Select a feature from the drop-down list to use its values as known concentrations. Feature values may be provided for all, some, or just a single sample. Any available information will be exploited by MCR. See Data Table Editor for how to add features to samples.
`Known spectrum`	Select a sample from the drop-down list to use its spectrum as known pure component spectrum.

Convergence

MCR-ALS is an iterative algorithm which uses convergence options as stopping criteria:

`Show intermediate results`	Enable to display graphical progress of component spectra and concentration profiles after each iteration.
`Maximum number of iterations`	The algorithm stops after the specified number of iterations.
`Maximum number of unsuccessful attempts`	The algorithm stops after the specified number of iterations without progress.
`Convergence tolerance`	The algorithm stops when the progress between iterations is below the specified tolerance.

Available Reports

Component Spectra
Spectra of identified pure components

Concentrations
Estimated concentrations (dimensionless)

RMS Spectral Residuals
Euclidean mean error of identified component spectra fitted linearly to measured samples

Table: Concentration Profiles
Numeric values of computed concentrations

Table: Component Spectra
Numeric values of pure component spectra

Report Customization

X-axis
By default, concentrations and RMSE values are plotted against the sample index. You can change the x-axis to any available sample feature. See Data Table Editor for how to add features to samples.

Component Selection
By default, plots of all pure component spectra and concentrations are shown in the graphical report. Use the list for selective plotting. Note that RMSE values are independent of the selected component.

More Iterations

You could conduct more iterations to improve results. When clicking **More Iterations** at the bottom of the Report Window, MCR-ALS starts again, letting you choose different constraints if desired, but using previous results as starting values.

3.8.4 HMFA

Menu bar:	Analysis > HMFA > Component Number Analysis
Menu bar:	Analysis > HMFA > Component Analysis

Hard Modeling Factor Analysis (HMFA) intends the recovery of pure component spectra and concentration profiles of the chemical constituents of a mixture when no prior information is available about the nature and composition of these mixtures. It is akin to other factor analysis methods, e.g., Multivariate Curve Resolution (MCR), but results are closer to physics due to the usage of Hard Models.

HMFA is performed for the selection in the Samples Panel, not including samples with `Quality = Bad`. A Hard Model is required for this analysis.

The Hard Model of HMFA

The Hard Model in HMFA is used to provide the factor analysis with as much information as possible about the spectral structure of the mixture. E.g., if any pure component spectrum is known in advance, a corresponding component should be part of the Hard Model. All remaining peaks belonging to unknown components should be modeled in the first Hard Model Component. HMFA redistributes peaks of the first Hard Model Component to new components by analyzing the mixture spectra and identifying peaks that belong together.

If, for instance, all pure component spectra were unknown, you could initially create a Hard Model with all peaks contained in the first Hard Model Component and let HMFA reassign them to new components.

The identification of unknown component spectra works well if two requirements are met:

- The first Hard Model Component must contain all the relevant peaks. No peaks must be missing, because only existing peaks can be reassigned. For creating such a representative model, it is recommended to use a representative sample of the mixture spectra for modeling.
- The mixture spectra must contain reasonable variation in the components' concentrations.

Eventually, HMFA fits the new Hard Model (which now contains the newly identified components, and all initially provided components) to the mixture spectra to compute component weights. Note that this kind of component fitting differs from regular component fitting in the following aspects:

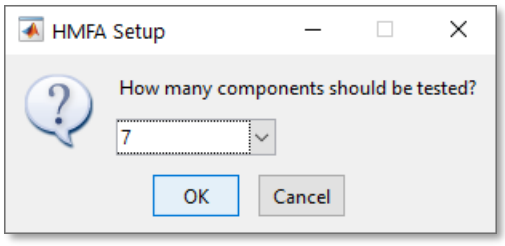
- The Hard Model is fitted linearly no matter the component fitting mode specified in the Hard Model settings.
- Fixed parameters are adjusted anyway.
- The Hard Model Baseline is ignored; instead, a linear baseline is fitted.

3.8.4.2 Component Number Analysis

Menu bar:	Analysis > HMFA > Component Number Analysis

Estimates the number of unknown mixture constituents by means of different figures of merit. A Hard Model with at least 2 peaks in the first component is required for this analysis. Results are displayed in a Report Window. Additional input is required for this analysis.

Setup



`Components to test`	The maximum number of components to get tested. HMFA is performed for each number from 1 to the selected maximum.

Available Reports

Average RMS Residuals of Component Fits
The average RMS residuals of component fits is the best indicator for determining the component number because it is an a-posteriori figure of merit. A-posteriori means that a model is created for each number of components and then an assessment is made of how well it explains the data by averaging the RMS residuals across all samples. The most likely number is reached when the next component does not significantly reduce the average RMS residuals anymore. Note that the diagram also displays a vertical line which is an estimate of the lower bound.

Explained Variance
Each component contributes to explaining the variance of the %s data matrix. The most likely number of components is reached when the next component does not significantly increase the explained variance anymore.

Ratios
The ratios plot supplements the Average-RMS-residuals-plot and the Variances-plot by showing the ratios of two successive RMS-values and variances, respectively. The most likely number of components is indicated by a large ratio.

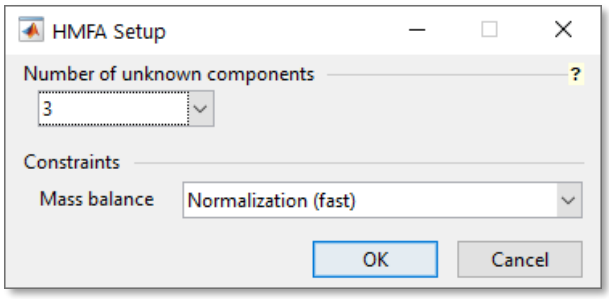
Factor Indicator Function
The factor indicator function reaches a minimum where the correct number of factors/components is expected. However, this only occurs when the error is random and uniform throughout the entire data. [E. R. Malinowski, Analytical Chemistry, Vol. 49 (4), April 1977]. In real cases, the function is typically L-shaped for about the first 10 components and the most likely number of components is indicated by a sharp bend in the curve.

3.8.4.3 Component Analysis

Menu bar:	Analysis > HMFA > Component Analysis

Identifies unknown component spectra (if any) and component concentrations from a set of mixture spectra. Results are displayed in a Report Window. Additional input is required for this analysis.

Setup

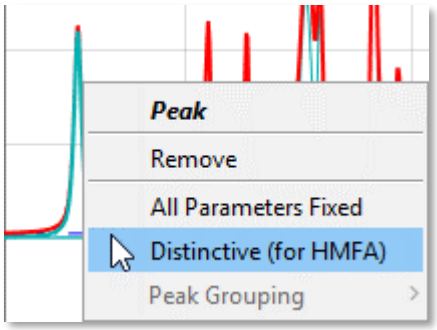


`Number of unknown components`

The number of components to be identified. The following options are possible:

`Integer >= 1`. Available if the Hard Model's first component contains peaks. The selected number of components will be identified.

`Auto`. Available if the Hard Model's first component contains peaks tagged as **Distinctive (for HMFA)**. A separate component will be identified for each distinctive peak, using the distinctive peak as a reference peak.



`0 (Zero)`. Available as the only option if the Hard Model's first component does not contain peaks. No unknown components can be identified in this case. HMFA will simply perform a linear fit of all Hard Model Components.

`Mass balance`

The option for post-processing of calculated component weights:

`None`. Computed component weights are not processed any further.

`Normalization`. For each sample separately, computed component weights are normalized such that the sum of weights will be one.

	`Optimization`. For all samples simultaneously, computed component weights are multiplied by common factors which are found by numerical optimization. Again, the sum of weights will be one for each sample.

Available Reports

Component Spectra
Spectra of all identified pure components (if any) and all initially provided pure components (if any)

Concentrations
Calculated component weights processed according to chosen closure constraint. If no closure constraint is applied, these values are in fact component weights. Otherwise, values represent dimensionless concentrations.

RMS Spectral Residuals
Euclidean mean of differences between fitted model and measured samples

Table: Concentration Profiles
Numeric values of computed concentrations

Table: Component Spectra
Numeric values of pure component spectra

Report Customization

X-axis
By default, concentrations and RMSE values are plotted against the sample index. You can change the x-axis to any available sample feature. See Data Table Editor for how to add features to samples.

Component Selection
By default, plots of all pure component spectra and concentrations are shown in the graphical report. Use the list for selective plotting. Note that RMSE values are independent of the selected component.

Create Hard Model

If at least one unknown component gets identified, you can export the components as a new Hard Model. Clicking the **Create Hard Model** button adds a new Hard Model to the Model Tree Panel which contains all identified components.

3.8.5 Integration

Menu bar:	Analysis > Integration

Calculates component areas by numerical integration of spectra. Results are displayed in a Report Window.

Integration is performed for the selection in the Samples Panel, not including samples with `Quality = Bad`. An Integration Model is required for this analysis.

Available Reports

Peak Area
Calculated peak areas

Report Table
Table with numeric peak areas

Report Customization

X-axis
By default, peak areas are plotted against the sample index. You can change the x-axis to any available sample feature. See Data Table Editor for how to add features to samples.

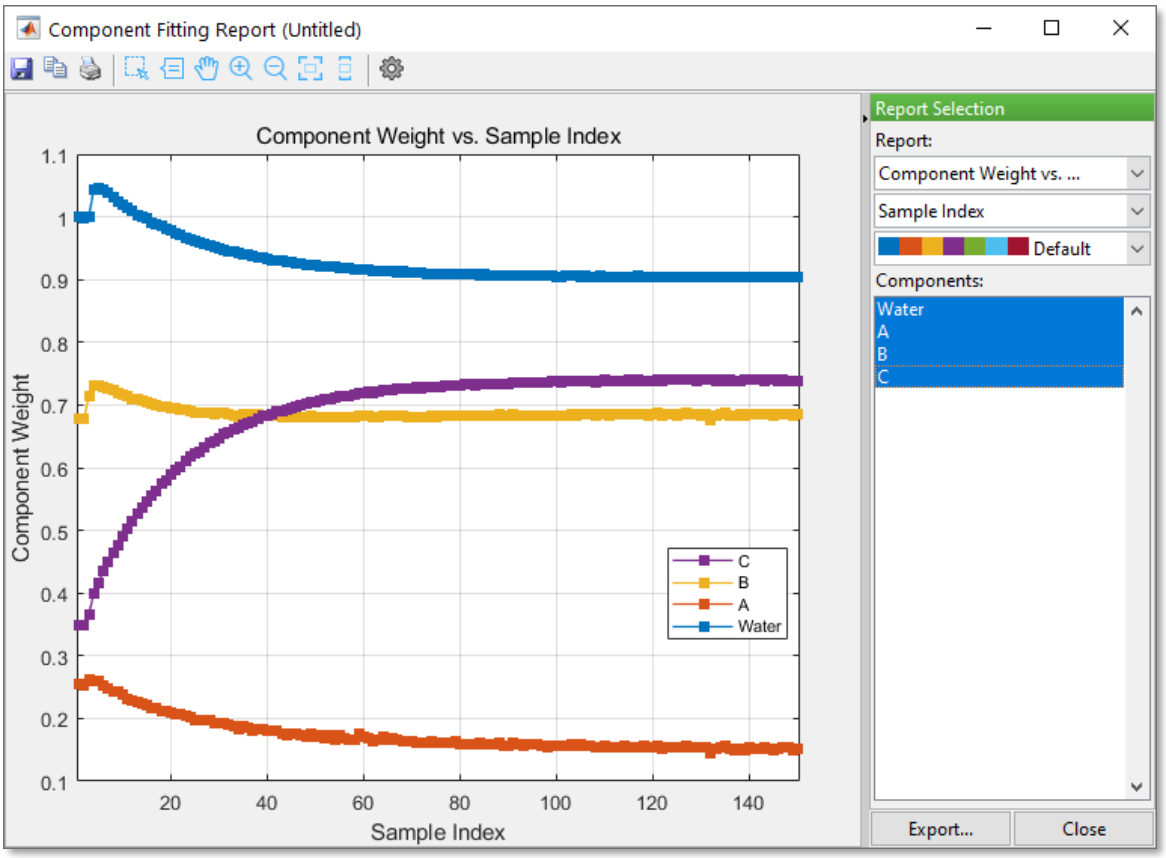
Component Selection
By default, plots of all Integration Model Components are shown in the graphical report. Use the list for selective plotting.

3.8.6 Component Fitting

Menu bar:	Analysis > Component Fitting

Calculates component weights and other figures of merit by fitting a Hard Model to sample spectra. Component fitting is performed according to the specifications of the Hard Model. Results are displayed in a Report Window.

Component fitting is performed for the selection in the Samples Panel, not including samples with `Quality = Bad`. A Hard Model is required for this analysis.



Available Reports

Component Weight
Calculated component weights

Component Area
Calculated component areas. Whether this report is available depends on preferences.

RMS Spectral Residuals
Euclidean mean of differences between fitted model and measured samples

Table: Component Report
Table with numeric component weights, component areas, and RMSE values. Whether or not the report contains component areas depends on preferences.

Table: Parameter Report
Table with numeric values of all parameters of all Component Fits

Report Customization

X-axis
By default, component weights and RMSE values are plotted against the sample index. You can change the x-axis to any available sample feature. See Data Table Editor for how to add features to samples.

Component Selection
By default, plots of all Hard Model Components are shown in the graphical report. Use the list for selective plotting. Note that RMSE values are independent of the selected component.

Component Fit Preview

Toolbar:	 (preview linear Component Fit)
Menu bar:	Analysis > Manage Fits > Preview Linear Fit
or	
Toolbar:	 (preview Component Fit according to model settings)
Menu bar:	Analysis > Manage Fits > Preview Component Fit

The Component Fit preview mode can be used to visually inspect the goodness of Component Fits in the main window. A Hard Model is required, and a sample must be active to enable the preview mode.

You can either display a linear Component Fit or the actual Component Fit as specified in the model setting. The former one is just provided for a quick preview; the latter is the important one and is typically referred to when speaking of Component Fits.

When the Component Fit preview mode is enabled, the Properties Panel displays properties of the Component Fit instead of the original Hard Model and the Plot Panel shows the Component Fit, i.e., the fit of the original Hard Model to the active sample.

Note: Some model parameters cannot be modified while in preview mode.

Managing Component Fits

Since component fitting could be a time-consuming operation, calculated fits will be stored in memory. All samples having Component Fits available are labeled with [C] in the Samples Panel. When the preview mode is enabled, a new Component Fit will be computed automatically for the active sample if none exists.

Component Fits will be removed from memory, when

- modifying the Hard Model.
- removing fits manually via menu Analysis > Manage Fits > Remove ...
- shutting down PEAXACT. You could save the session to preserve all Component Fits for the next time.

Component Fits can be stored permanently, when

- saving the session
- exporting the current Component Fit as new Hard Model to a model file via menu Analysis > Manage Fits > Export Visible Fit as New Model...

3.8.7 Prediction

Menu bar:	Analysis > Prediction

Calculates feature values and other figures of merit from spectra using a Calibration Model. Results are displayed in a Report Window.

Prediction is performed for the selection in the Samples Panel, not including samples with `Quality = Bad`. A Calibration Model is required for this analysis.

Available Reports

Predicted Feature
Predicted feature values are plotted against a selectable feature. Error bars represent the prediction uncertainty for a 95% level of confidence.

RMS Spectral Residuals
The Root Mean Squared Spectral Residuals measure how well the model explains the spectral data. RMSE values are only shown for samples for which reference values are provided. See also calibration reports.

Mahalanobis distance
The Mahalanobis Distance tells how well a sample matches the training samples used for calibration. The Mahalanobis Distance can be used to spot spectral outliers. See also calibration reports.

Report Table
Table with numeric values of predicted features.

Report Customization

X-axis
By default, predicted features are plotted against the sample index. You can change the x-axis to any provided sample feature. See Data Table Editor for how to add features to samples.

Component Selection
By default, plots of all Calibration Model Components (features) are shown in the graphical report. Use the list for selective plotting.

Command Line Alternative

Predictions can also be started from the command line with option `-predict`. This has advantages over the graphical user interface:

- Simultaneous analysis with multiple models
- Results of all models are combined in a single report file
- Results will not be lost in case of a system crash
- Less memory-intensive
- Suited for analyzing many samples

Predictions are performed for all loaded samples using all opened calibrated models. To load models and samples from the command line, you could:

- save a session file in advance which contains all your necessary models and samples; then use command line options `-restore` or `-session <file>` in addition to `-predict`
- load additional files directly from the command line by adding filenames to the command, e.g., `peaxact -predict "my model.pxm" c:\data\dataTable.xls`

Results are written to a spreadsheet
`%LocalAppData%\S-PACT\PEAXACT 5\Reports\<YYYY-MM-DD hh.mm.ss> Analysis.csv`.

> Note: Results are written to file directly after the analysis of each sample, i.e., results will not get lost in case of a system crash.

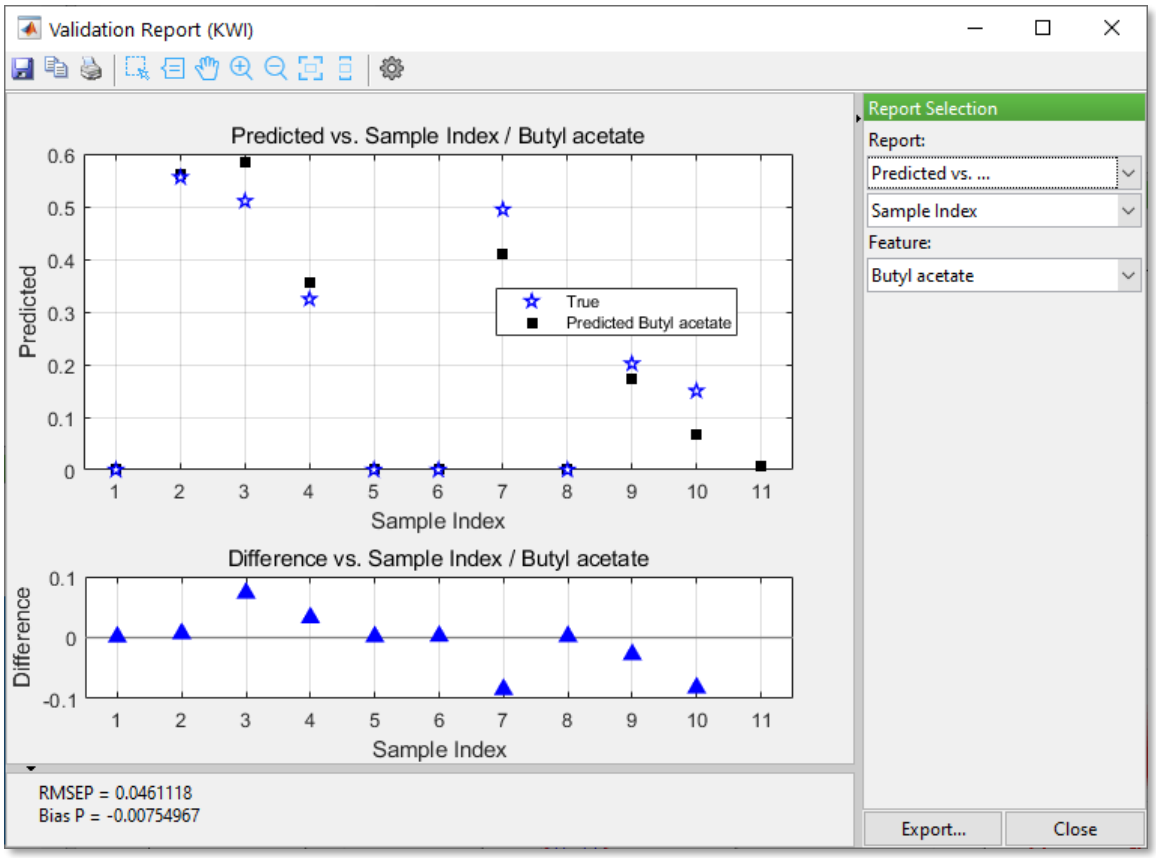
See also: Command Line Options

3.8.8 Validation

Menu bar:	Analysis > Validation

Calculates feature values and other figures of merit from spectra using a Calibration Model and compares predicted values with available reference values. Results are displayed in a Report Window.

Validation is performed for the selection in the Samples Panel, not including samples with `Quality = Bad`. A Calibration Model is required for this analysis. Selected samples should (but do not have to) provide values for calibrated features which could be used as reference values for quantitative validation of the model's predictive capabilities.



The Validation Report Window displays values from three different sources:

- Predicted feature values of selected samples. Values are shown independently for each feature (and for each group in case of a groupwise calibration/prediction), i.e., each feature (and group) can be validated separately.
- Reference values of selected samples. See Data Table Editor for how to add features to samples.
- Reference values of training samples used during calibration. This is useful for comparing newly predicted values with original training data.

Available Reports

Predicted vs. True
Predicted feature values are plotted against the actual values for each sample for which such reference value is provided. In addition, reference values used during calibration are displayed for comparison.

Predicted vs. ...
Predicted feature values are plotted against a selectable feature. Error bars represent the prediction uncertainty for a 95% level of confidence. In addition, for each sample for which reference values are provided, a marker represents the actual value, and differences between predicted and actual values are shown in a second graph.

RMS Spectral Residuals vs. True
RMS Spectral Residuals vs. …
The Root Mean Squared Spectral Residuals measure how well the model explains the spectral data. RMSE values are only shown for samples for which reference values are provided. See also calibration reports.

Mahalanobis distance vs. True
Mahalanobis distance vs. RMS Spectral Residuals
Mahalanobis distance vs. …
The Mahalanobis Distance tells how well a sample matches the training samples used for calibration. The Mahalanobis Distance can be used to spot spectral outliers. See also calibration reports.

Report Customization

X-Axis
For some reports, you can change the x-axis to any provided sample feature. See Data Table Editor for how to add features to samples.

Component Selection
Use the drop-down list to display results for individual Calibration Model Components (features).

Group
Use the drop-down list to display results for individual groups (available for groupwise calibration/prediction only).

3.8.9 Identification

Menu bar:	Analysis > Identification

Calculates feature classes and other figures of merit from spectra using a Classification Model. Results are displayed in a Report Window.

Identification is performed for the selection in the Samples Panel, not including samples with `Quality = Bad`. A Classification Model is required for this analysis.

Available Reports

Identified Class
Identified classes.

Report Table
Table with identified class names and class probabilities.

Report Customization

X-axis
By default, identified classes are plotted against the sample index. You can change the x-axis to any available sample feature. See Data Table Editor for how to add features to samples.

3.8.10 Custom

Menu bar:	Analysis > Custom

Calculates custom results from spectra using a Custom Model. Results are displayed in a Report Window.

The analysis is performed for the selection in the Samples Panel, not including samples with `Quality = Bad`. A Custom Model is required for this analysis.

Available Reports

Numerical Results
Values of numerical custom results.

Report Table
Table of all Custom Results (numerical and categorical).

Report Customization

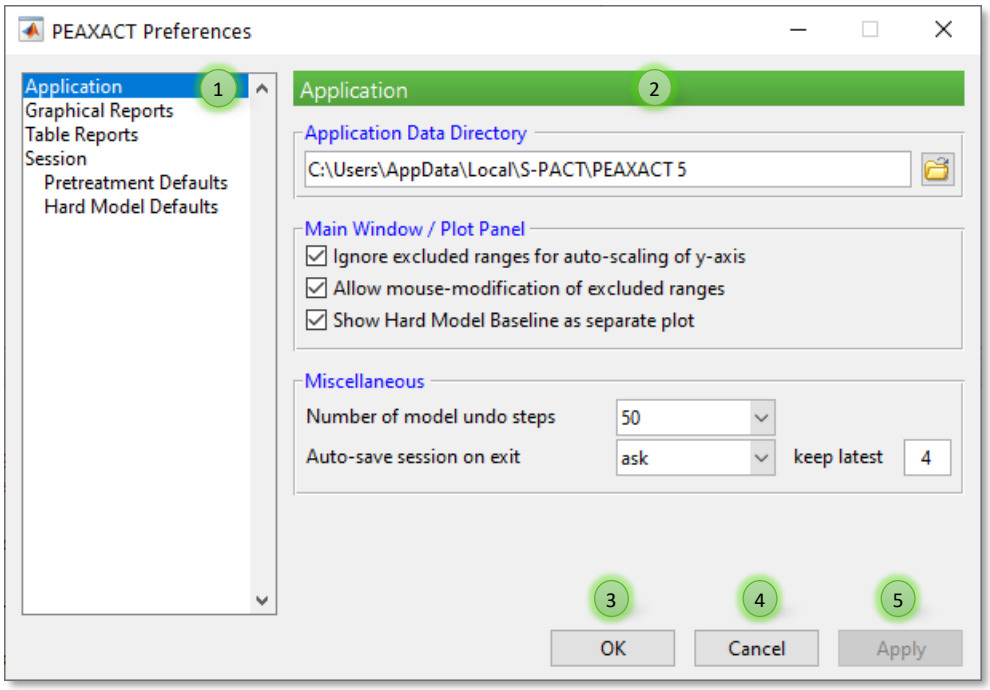
X-axis
By default, calculated values are plotted against the sample index. You can change the x-axis to any available sample feature. See Data Table Editor for how to add features to samples.

3.9 Preferences

3.9.1 Preferences Editor

Menu bar:	File > Preferences
Toolbar:	
Status bar:	Left-click on session profile name

Use the Preferences Editor to adjust PEAXACT settings.



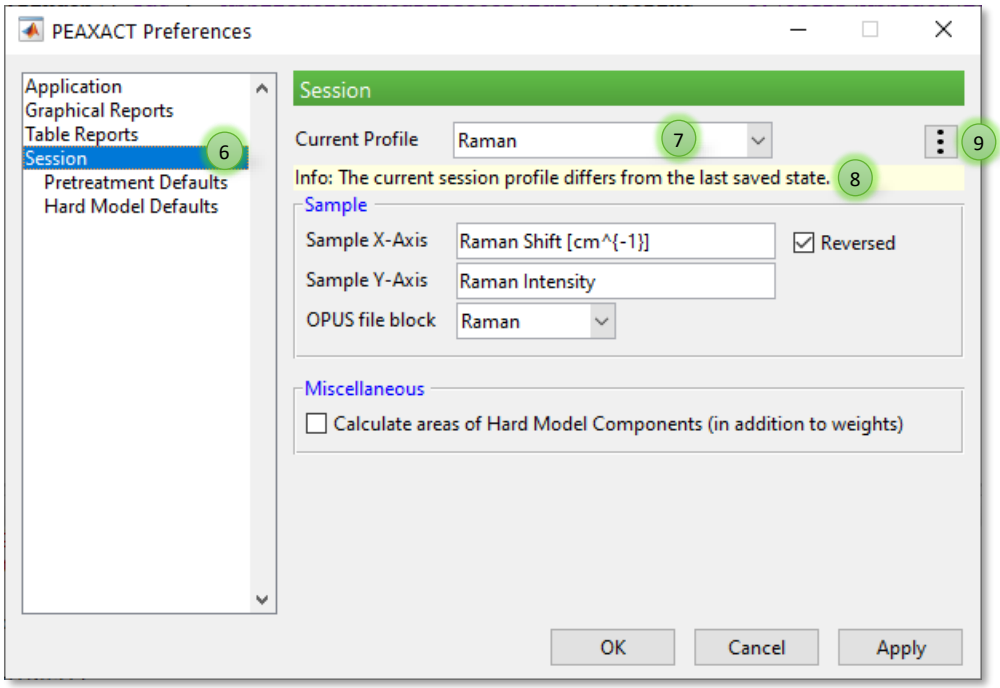
Preferences Editor

1) Select a category
2) Edit preferences of selected category
3) Apply changes and close dialog
4) Discard changes and close dialog
5) Apply changes without closing the dialog

Changing Preferences

Choose a category from the list (1) and then change preferences using the controls in the right pane (2). Click the OK (3) or Apply (5) button to accept changes; click the Cancel (4) button to discard changes.

Changing the Session Profile



6) Session preferences
7) Select a session profile
8) Information about the profile
9) More options for resetting, saving, or deleting the profile

Session-related preferences are stored in profiles. There are several profiles for different purposes but only one profile can be active at a time.

After selecting the Session category (6) use the drop-down list (7) to select a profile and load its preferences into the editor. Click the OK or Apply button to accept the loaded session preferences.

Change session preferences using the controls in the right pane. The info bar (8) tells you when the current session profile has changes. If you want to reset or save those changes, click button (9) to call up the context menu with more options. If you select another profile while the current one has changes, you will be asked whether you want to save changes first.

> Note: You do not have to save profile changes. It is enough to click the OK button to accept all changes.

Reset, Save, Create, or Delete Session Profile

Click the button (9) to call up the context menu with more options for the current session profile:

`Reset to Last Saved State` Reload the profile from its file

`Reset to Factory Defaults`	Available only for pre-defined profiles
`Save as "<name>"`	Save changes under its current name
`Save as…`	Save the profile under a new name
`Delete`	Available only for user-created profiles

Note: Saving a profile does not automatically accept the new preferences. You still must click the OK button.

3.9.2 Application Settings

Application Data Directory

PEAXACT uses a special application data directory to save files at runtime. The directory cannot be changed, but for your convenience it is displayed in the Preferences Editor and can be opened in the Windows explorer by clicking the button next to the field.

Main Window / Plot Panel

`Ignore excluded ranges for auto-scaling of y-axis`	The option to specify scaling of the y-axis.
	`Enabled`. Y-axis limits are adjusted automatically to fit only the relevant measured signal, i.e., any signal that is not excluded.
	`Disabled`. The y-axis is scaled automatically to fit the full measured signal.
`Allow mouse modification of excluded ranges`	Excluded ranges are displayed as gray patches in the Plot Panel. These patches typically overlap other plots. This option specifies the behavior when clicking on an excluded range patch.
	`Enabled`. Excluded range patches could be modified interactively using the mouse. In this case it may be difficult to interactively modify other plots which are overlapped by patches.
	`Disabled`. Excluded range patches cannot be modified interactively. Instead, it is easier to click and modify plots which are overlapped by patches.
`Show Hard Model Baseline as separate plot`	The option for how to treat the plot of the Hard Model Baseline.

	`Enabled`. A separate plot for the Hard Model Baseline is displayed in the Plot Panel. The plot can be used to interactively modify the baseline.
	`Disabled`. The Hard Model Baseline is still calculated but it is not displayed as a plot. Instead, the baseline gets subtracted from the active sample and the corrected sample is displayed in the Plot Panel. This needs to get used to but has the advantage of the sample signal being shifted towards zero, which is favorable for Hard Modeling in case of strong baseline signals.

Miscellaneous

`Number of model undo steps`	The number of modeling steps that can be undone.
`Auto-save session on exit`	This option specifies whether the current session is saved to the auto-save directory when exiting PEAXACT.
	`Never`. The current session is not saved.
	`Ask`. The user is asked whether to save the session.
	`Always`. The current session is saved automatically.
`Keep latest N`	The number of session files to keep in the auto-save directory. Only the N most recently saved sessions are kept.

3.9.3 Graphical Report Settings

Graphics Style

`Font Style`	The font family, font decoration, and font size for text in graphical reports.
`Plot Style`	Options for showing/hiding the title, axis labels, axis ticks, legend (if any), and error bars (if any) of graphical reports.

Export

`Image export resolution (DPI)`	This option only applies when exporting images to a file.
	`Auto`. A default resolution for exporting graphical reports to file. The actual value depends on the output file format.

	`72, 100, 150, 200, 300, 600`. A fixed resolution (in dots per inch) for exporting graphical reports to a file. A larger value improves image quality, but also increases file size.
`Image export to clipboard`	This option only applies when copying images to the clipboard.
	`Rendered`. Graphical reports are copied as raster images (bitmaps).
	`Vector`. Graphical reports are copied as vector images.

3.9.4 Table Report Settings

Table Style

`General report information at the top`	The option to include general information in table reports.
	`Enabled`. Tabular reports start with a few rows containing general information like the report creation time or the model file the analysis is based on (if any).
	`Disabled`. The report consists of analysis results only.
`Include sample features`	The option to include sample features in table reports.
	`Enabled`. The report's result table is expanded to the right to also include all available features of the samples being analyzed.
	`Disabled`. The report consists of analysis results only.
`Timestamp first`	The option to include sample timestamps at the beginning of table reports.
	`Enabled`. Timestamp values are treated in a special way and, if available, are added as first column to the left of result values.
	`Disabled`. Timestamp values are treated like other feature values.

Export

`Delimiter character for CSV files`	The character to be used as delimiter when saving comma separated value (CSV) files.

3.9.5 Session Settings

Sample

`Sample X-Axis`	The label for the independent x-variable of the sample signal; may contain simple TeX expressions.
`Sample Y-Axis`	The label for the dependent y-variable of the sample signal; may contain simple TeX expressions.
`Reversed`	The option to specify the direction of the x-axis.
	`Enabled`. The sample x-axis is displayed reversed (right-to-left). This is characteristic for spectra.
	`Disabled`. The sample x-axis is displayed normally (left-to-right). This is characteristic for chromatograms and NMR FID signals.
`Default OPUS file block`	The filter for data blocks read from Bruker OPUS files. If the file does not contain the default block all blocks get loaded instead.

Miscellaneous

`Calculate areas of Hard Model Components`	The option to specify whether Hard Model Component areas should be calculated.
	`Enabled`. For Hard Models, the contribution of components to a mixture is typically expressed in terms of component weights (relative component areas). When this option is enabled, absolute component areas are calculated in addition to component weights and displayed next to weights in reports.
	`Disabled`. No calculation of Hard Model Component areas.

Pretreatment Defaults

Pretreatment defaults represent default settings for new models. Whenever a new model is created, its Pretreatment Model gets initialized with values taken from the then-current session profile. For a description of individual settings, see Pretreatment Model.

Hard Model Defaults

Hard Model defaults represent default settings for new Hard Models. Whenever a new Hard Model is created, its settings get initialized with values taken from the then-current session profile. For a description of individual settings, see Settings for Hard Model Fitting.

3.10 License Management

Menu bar:	Help > Licensing...

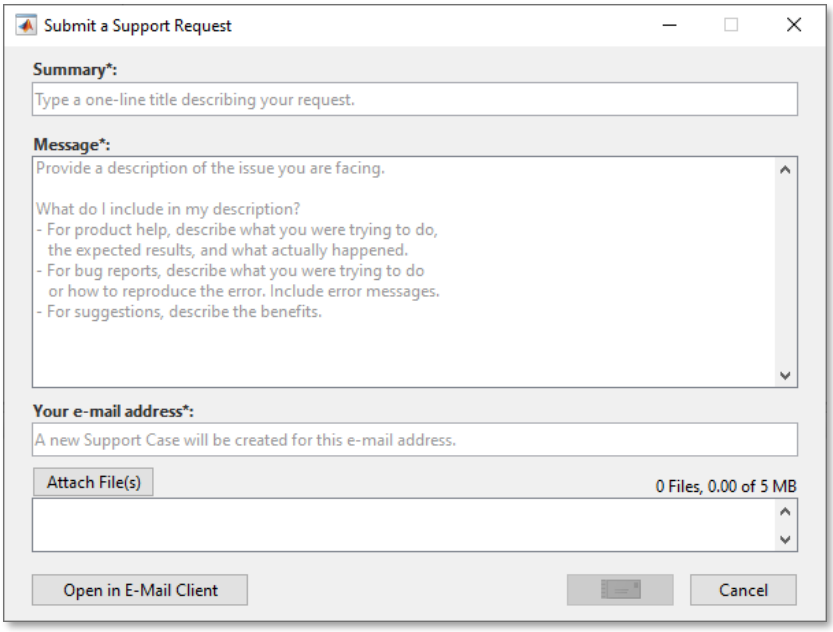
Use the License Activation Dialog to change your license if required (see License Activation). The License Activation Dialog also displays information about the current license.

3.11 Technical Support

3.11.1 Request Support

Menu bar:	Help > Request Support...

Use the Support Request Dialog to send e-mails to S-PACT Technical Support directly from within PEAXACT.



You may want to send support requests for different purposes, e.g.:

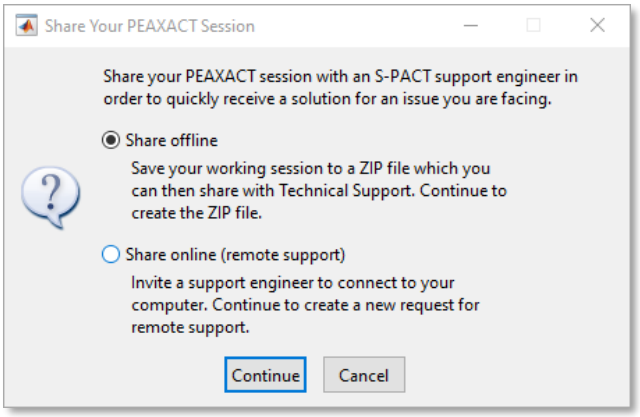
- asking for help
- reporting a bug / crash
- suggesting new features
- giving any kind of feedback

In each case, provide a subject and description of the issue with which you are facing. You can optionally attach related files, e.g., a screenshot or a session file. When clicking the **Send** button, an e-mail is sent to support@s-pact.com, creating a new support case. If your computer is currently offline or uses protective methods to restrict internet access, click the **Open in E-Mail Client** button to have the mail sent by your default e-mail application.

3.11.2 Share Session with Technical Support

Menu bar:	Help > Share...

You can share your PEAXACT session with an S-PACT support engineer to get a solution for an issue you are facing.



`Share offline`	Save your working session to a ZIP file which you can share then with Technical Support. Click **Continue** to create the ZIP file and open the Support Request Dialog to optionally create a new support case. Note: Technical Support can provide you with a secure upload link for large files.
`Share online`	Invite an S-PACT support engineer to connect to your Windows desktop. You can show your working session on your computer as if a support engineer were sitting right next to you. Click **Continue** to open the Support Request Dialog and request remote support.

4 TROUBLE SHOOTING

Graphics problems

Symptoms
Some windows such as the main window or the Data Inspector are not displayed correctly, e.g., showing upside-down text, duplicated text, misplaced axes tick labels, black bars, or scrambled graphics.

Cause
Problems are related to hardware-based graphics acceleration performed by some video cards.

Resolution
Make sure to use the newest version of drivers for your graphics card. If the problem suddenly occurs after you updated the drivers, revert to a previous version of drivers.

Start PEAXACT with command line option `-openglfix`. This forces the usage of software-based graphics acceleration. You should only use this command line option if you encounter graphical problems because software-based acceleration is typically slower than hardware-based acceleration.

- Right-click the Windows Desktop and choose **New > Shortcut**
- Enter
  `"C:\Program Files\S-PACT\PEAXACT 5\Peaxact.exe" -openglfix`
  You may need to replace the directory with the PEAXACT installation directory on your computer. Do not forget the double quotes.
- Click **Next** and enter a shortcut name.
- From now on start PEAXACT using the new shortcut.

Startup error: Missing MWArray

Symptoms
The following error is displayed during PEAXACT startup:
Could not load file or assembly 'MWArray, Version=2.19.0.0 [...]' or one of its dependencies.

Cause
`MWArray.dll` (Version 2.19.0.0) is part of MATLAB Runtime 2019a and is in the Windows global assembly cache (GAC). The error occurs when the file is missing in the GAC, probably because of a missing or incomplete installation of MATLAB Runtime 2019a.

Resolution
Perform a clean installation of PEAXACT. This will also install MATLAB Runtime 2019a including `MWArray.dll`.

- Uninstall PEAXACT
- Uninstall MATLAB Runtime 9.6
- Delete all remaining files from the MATLAB Runtime installation directory:
  `C:\Program Files\MATLAB\Matlab Runtime\v96`
- Reboot the computer.

- Install PEAXACT again.

Startup error: Type initializer for MathWorks.MATLAB

Symptoms
The following error is displayed during PEAXACT startup:
The type initializer for 'MathWorks.MATLAB [...]' threw an exception.
Caused by:
E.g.: Failed to find mclmcrrt9_6.dll required to load dotnetcli on system path [...]

Cause
`mclmcrrt9_6.dll` is part of MATLAB Runtime 9.6 and is in the MATLAB Runtime installation directory. The file path is added to the system's PATH variable. The error either indicates that the file is missing from the installation directory, or that the file path is missing from the PATH variable.

Resolution
Check whether the system's PATH variable contains the following entry:
`C:\Program Files\MATLAB\Matlab Runtime\v96\runtime\win64`
If missing, consider adding it to the PATH variable.

- Press [Windows Key] + R (or select start menu > Run...)
- Type: `rundll32.exe sysdm.cpl,EditEnvironmentVariables`
  This opens the editor for environment variables.
- In the upper half of the window, double-click the variable named **Path**, select **New**, and add `C:\Program Files\MATLAB\Matlab Runtime\v96\runtime\win64` to the list.

Alternatively, a clean installation of PEAXACT should fix the problem. This will also install MATLAB Runtime 9.6 including `mclmcrrt9_6.dll`.

- Uninstall PEAXACT
- Uninstall MATLAB Runtime 9.6
- Delete all remaining files from the MATLAB Runtime installation directory:
  `C:\Program Files\MATLAB\Matlab Runtime\v96`
- Reboot the computer.
- Install PEAXACT again.

Startup error: MATLAB Runtime instance

Symptoms
The following error is displayed during PEAXACT startup:
The MATLAB Runtime instance could not be initialized.

Cause 1
During startup, PEAXACT extracts files to a MATLAB Runtime cache directory defined by a system environment variable named `MCR_CACHE_ROOT`. The error occurs when files cannot be read from the directory, e.g., due to partially missing or corrupted files.

Resolution 1
Delete the cache directory:

- Browse to the cache directory by typing the following into the address bar of the Windows Explorer:
  `%MCR_CACHE_ROOT%`
- Delete all files and folders within the cache directory.

Restart PEAXACT

Cause 2
The error also occurs when files cannot be written to the `MCR_CACHE_ROOT` directory, e.g., due to missing write permissions.

Resolution 2
Consider relocating the cache directory:

- Press [Windows Key] + R (or select start menu > Run…)
- Enter: `rundll32.exe sysdm.cpl,EditEnvironmentVariables`
  This opens the editor for environment variables.
- In the upper half of the window, select **Create…**, then enter
  Variable name: `MCR_CACHE_ROOT`
  Variable value: `%LocalAppData%\MatlabRuntime`

You may want to substitute the variable value by a different path for which you have full access permissions.
Startup error

Other Problems

If you encounter a problem not mentioned before, try the following:

- Start PEAXACT using the `PEAXACT 5 Debugging` shortcut in the PEAXACT installation directory `C:\Program Files\S-PACT\PEAXACT 5`. This enables verbose logging.

Send the log file to support@s-pact.com and request help from Technical Support.

5 LITERATURE

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