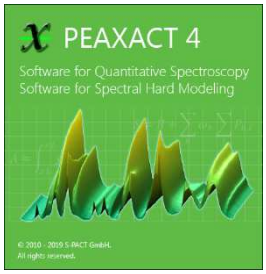
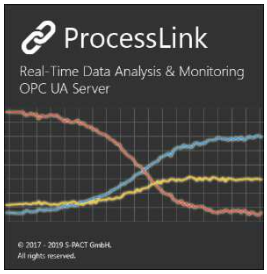
PEAXACT – Software Overview





Key Issues

- PEAXACT Key Features
- Spectral Hard Modeling – PEAXACT USP
- Unsupervised analysis with Application Server
- PEAXACT ProcessLink – universal link into process

Overview

PEAXACT is an interactive chemometrics software for the creation of models (methods) for the quantitative multivariate analysis of spectra of all kinds: UV-VIS, infrared, Raman, NMR and beyond.

It covers all steps of data visualization and modeling in a unified workflow: data pretreatment, spectral modeling with mechanistic and statistical methods, and calibration. PEAXACT addresses to first-time users of quantitative spectroscopy as well as to experienced users who want to have access to a balanced spectrum of analysis methods.

Scheme 1: Full modeling workflow in PEAXACT.

Features for visual data inspection

The PEAXACT Data Inspector is a graphical tool for the editing and visualisation of spectra (Figure 1).

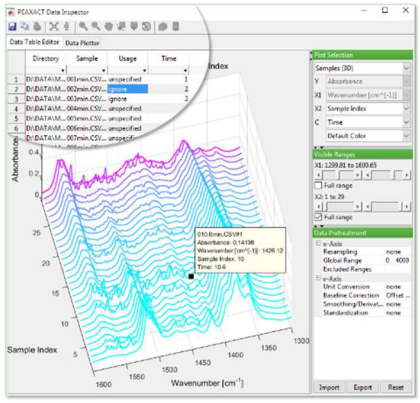


Fig. 1: Table and plot view in the Data Inspector.

Data inspection is supported by the following features:

- Organisation of spectra + reference data
- Customizable plots: 2D, 3D, 4D (color-coded)
- Principal Component Analysis (PCA)
- Export of images: PNG, JPEG, PDF, EPS, …

Options for Data Pretreatment

PEAXACT allows spectra pretreatments in manifold ways. All steps are applied in a physically meaningful order and prevent the user from nonsensical use.

1) Region selection (global and local)
2) Resampling: thinning, various interpolations
3) Baseline handling: offset, linear trend, rubber band
4) Smoothing, 1st and 2nd derivatives with smooth noise-robust differentiator (SNRD)
5) Standardization: maximum, area, SNV, peak

All data manipulations are immediately visualised on-the-fly and do not generate data set clones.

Spectral Modeling methods

PEAXACT provides a comprehensive toolbox for the quantitative analysis of spectra. A focus is on the so-called mechanistic methods using physically motivated quantification approaches.
PEAXACT's uniqueness lies in spectral **Hard Modeling**, a method using the physics of a mixture spectrum to

- Explain the spectrum shape by flexible peak curves that compensate mixture effects like position or shape changes and
- Explain the mixture composition by scaling these curves group-wise (component-wise).

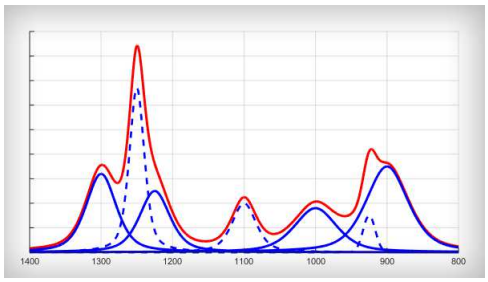


Fig. 2: Mixture Hard Model (red) with underlying components (blue), each a sum of peak functions.

Hard Modeling methods exploit the full physical knowledge about a mixture spectrum, including molecular interactions, temperature influence, meaning

that these models can be extremely **robust and hence ideal for process analytics**. Maintenance of these models is facilitated thanks to **clear diagnosis and error detection**.
Hard Models can be trained on few reference samples and thus **reduce calibration costs dramatically**. They even bear the chance to calibrate on partial mixtures only, e.g. in case of reactive mixtures or instable intermediates.
PEAXACT also supports Peak Picking, Band Integration, Peak Deconvolution and Multivariate Curve Resolution (for Multivariate Regression see below).

Calibration in PEAXACT

PEAXACT supports both **univariate and multivariate regressions**. Mechanistic models (Integration and Hard Models) are easily regressed in a univariate way, plus ratiometric regression for relative concentrations. PLS – **Projection to Latent Structures or Partial Least-Squares** – is available for multivariate regressions. Both test-set and cross-validation (leave-out, k-fold, group-wise) can be applied to estimate model performance. PEAXACT provides comprehensive reporting for selecting the best calibration alternative:

- RMSE(P,CV,C) and R^2 vs function/Rank
- Predicted vs True (recovery)
- RMS Spectral Residuals and Mahalanobis Distance plus outlier probabilities

Reports are provided both graphically and numerically.

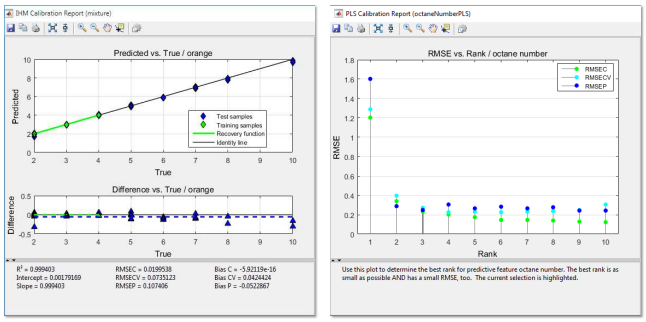


Fig. 3: Graphical reports for calibration selection.

All PEAXACT models can be used for interactive analysis of unknown spectra in PEAXACT directly.

Application Server (API)

Application Server enables you to **embed PEAXACT analytical methods into third-party applications**. You can integrate PEAXACT with your own application or use it in combination with measurement software as back-end-analyzer for the real-time evaluation of spectra. Both COM and .NET connectivity are available. These applications are ready for PEAXACT:

- HoloPro (Kaiser Optical Systems)
- OPUS PROCESS (Bruker Optics)
- MultiSpec Pro II (tec5)
- Process Pulse II (CAMO)

PEAXACT ProcessLink

ProcessLink is an extension of the Application Server, linking PEAXACT-based analysis to any lab or process spectrometer in an easy-to-use Windows app:

1) Select spectra folder to be monitored.
2) Select PEAXACT model(s).
3) Get results written to a text file.
4) Display real-time trend chart.
5) Large display of latest numerical results.
6) Publish results on an integrated OPC-UA Server.

Fig. 4: Real-time trend chart and result table.

This easy workflow quickly turns any spectroscopic device into a process analyser.

PEAXACT Resources

Find out more about PEAXACT!

Product website: www.s-pact.com/peaxact
PEAXACT Blog: www.s-pact.com/blog
Contact Support: contact@s-pact.de