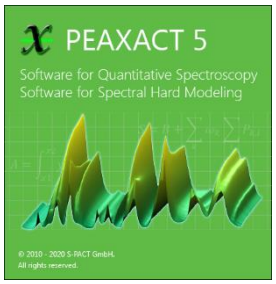
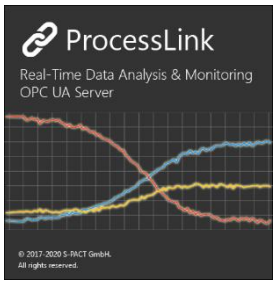
PEAXACT – Software Overview





Key Issues

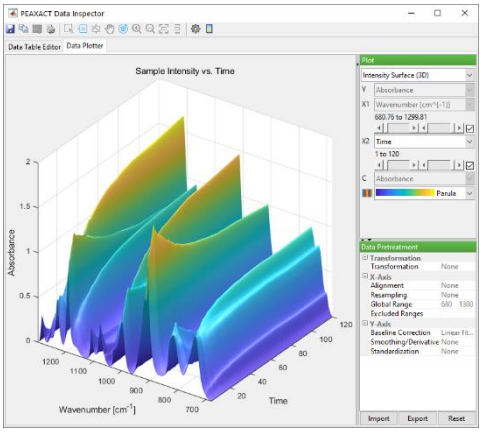
- Key Features of the PEAXACT Desktop App
- Spectral Hard Modeling – PEAXACT USP
- Integrated analysis with PEAXACT AppServer
- Side-by-side analysis with PEAXACT ProcessLink

Overview

The PEAXACT Desktop App 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. The software addresses to **first-time appliers** of quantitative spectroscopy and to **experienced experts** searching access to a balanced pool of methods.
PEAXACT supports the best-practice workflow of data analysis: visualization, exploration, data pretreatment, spectral modelling (mechanistical, statistical), training (calibration, classification), and post-processing.

Visual Data Inspection

The Data Inspector is PEAXACT's powerful graphical tool for the visualization and exploration of spectra and their numerical or categorical features.



Data Inspector.

- Organization of spectra and associated features
- Customizable plots: 2D, 3D, 4D (color-coded)
- Principal Component Analysis (PCA)
- Unsupervised Classification (Cluster Plot)
- Export of high-quality images

Data Pretreatment

PEAXACT provides a variety of pretreatments for spectra. All steps are applied in a physically meaningful order and prevent the user from nonsensical use.

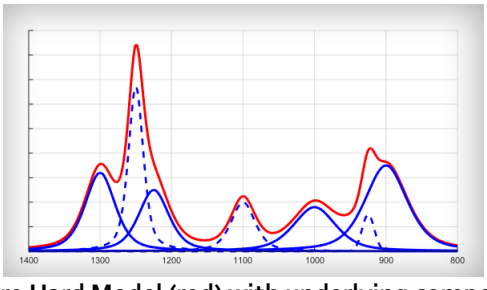
- NMR pre-processing: FT, phasing, zero filling
- Alignment
- Resampling: thinning, interpolation
- Range selection: global, local
- Baseline handling: offset, linear fit, rubber band
- Smoothing/derivatives (smooth noise-robust diff.)
- Standardization: maximum, area, SNV, peak

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

Spectral Modeling

PEAXACT provides a comprehensive toolbox for the quantitative analysis of spectra. A focus is on mechanistic methods using physically motivated models, particularly on spectral **Hard Modeling**, a unique 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).



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

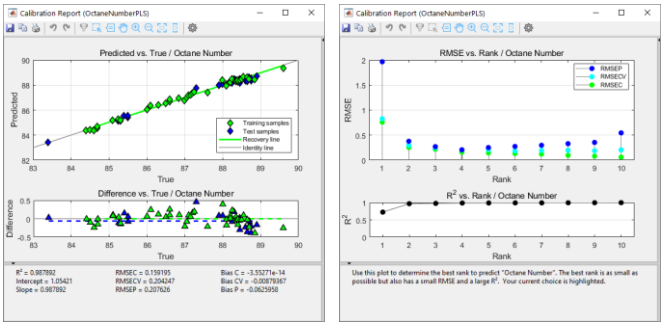
Hard Modeling methods exploit the full physical knowledge about a mixture spectrum, including molecular interactions, meaning that spectral Hard Models can

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 bear the chance to calibrate on partial mixtures only, e.g., in reactive mixtures or instable intermediates.
PEAXACT also provides other well-known spectral models such as classic band integration and principal components-based models.

Calibration and Classification

PEAXACT supports **univariate calibration** of mechanistic methods (Integration Models and Hard Models) and **multivariate calibration** for statistical methods (PLS/Projection to Latent Structures/Partial Least-Squares). A unique ratiometric regression is provided for correctly calibrating relative concentrations. For categorical features, PEAXACT offers different **classification methods**, from a simple database lookup to principal-component-based discriminant analyses.
Both test-set-validation and cross-validation (leave-out, k-fold, group-wise) are available to evaluate model performance. PEAXACT provides comprehensive reporting for finding the best calibration or classification alternative:

- RMSE and R^2 vs function/rank
- Predicted vs True
- Prediction uncertainties (error bars)
- Spectral residuals and Mahalanobis distances with outlier statistics



Graphical reports for evaluating calibrations.

All models can be used for interactive analyses of unknown spectra in the PEAXACT Desktop App directly.

PEAXACT AppServer

PEAXACT AppServer enables you to **embed PEAXACT analytical methods into third-party applications**.

Integrate PEAXACT with your own applications or use it in combination with measurement software as back-end analyzer for the real-time evaluation of spectra. Both **.NET** and **COM APIs** (application programming interfaces) are available. The following third-party applications are ready for PEAXACT:
RunTime (Endress+Hauser), SpectralSoft (Tornado), MultiSpec Pro II (tec5), SpinSolve (Magritek), synTQ (Optimal), Process Pulse II (AspenTech), SIPAT (Siemens), HoloPro (Kaiser Optical Systems).

PEAXACT ProcessLink

PEAXACT ProcessLink is an easy-to-use Windows App to link PEAXACT analyses to any lab or process spectrometer – no direct interface needed! It comes with an easy workflow:

- Select spectrum folders to be monitored.
- Select PEAXACT models.
- View results in a **real-time trend chart** or table.
- Access results from the **built-in OPC-UA server**.

Real-time trend chart and result table.

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

PEAXACT Resources

Product website	www.peaxact.com
Why PEAXACT?	www.peaxact.com/faq
PEAXACT Tour	www.peaxact.com/tour
Contact Support	contact@s-pact.com