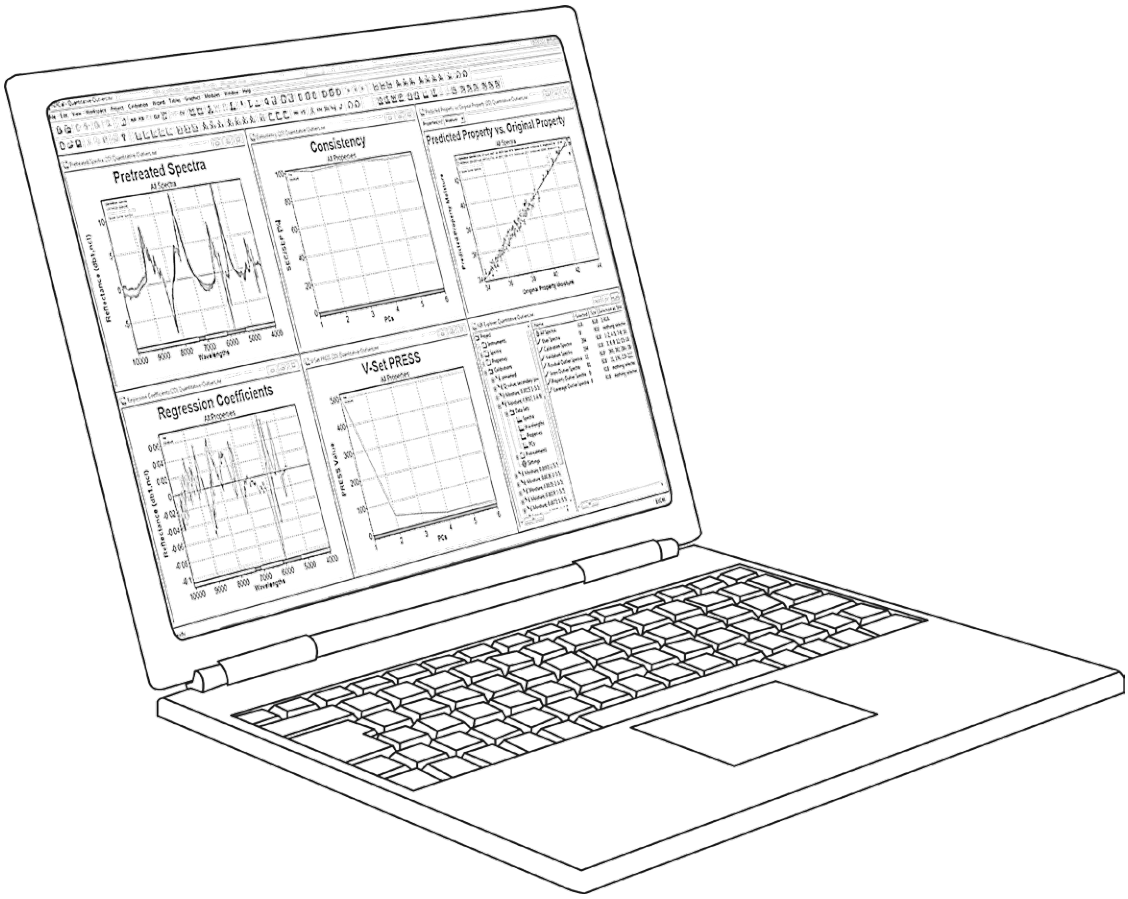
NIRCal
Software data sheet

NIRCal is an optional software package for NIRFlex N-500 and NIRMaster, that allows the development of qualitative and quantitative calibrations. It offers numerous chemometric algorithms, data pre-treatment and visualization tools to analyze your spectroscopic data. The patented Calibration Wizard automates the creation and optimization of precise and robust calibration models.



System requirements

The PC must fulfill the following requirements:

Operating System	Windows 10 Professional / Enterprise / Ultimate (64-bit) OR Windows 11 Pro / Enterprise (64-bit)
Central Processing Unit	Intel Core i3 or higher and 1.4 GHz or faster
RAM	4 GB or higher
Harddisk	20 GB free hard disk space
Display resolution	1280 x 1024
LAN	1 x 100 Mbit/s LAN (2 x 100 Mbit/s LAN recommend)
Others	DVD-ROM drive

Licenses

NIRCal	NIRCal chemometric software, including the Calibration Wizard (registration required)
NIRCal Toolbox	The Toolbox provides quick and easy access to the essential parameters, simplifying method development (specific license required)

Order code

Choose the configuration according to your needs:

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21 NIRCal 5 Chemometric Software CD incl. License
23 NIRCal 5 Chemometric Software CD - 3 Licenses
41 NIRCal Toolbox 1 CD incl. License (requires NIRCal)
42 NIRCal Toolbox 1 CD - 3 Licenses (requires NIRCal)

Functional principle

Workflow

The following table depicts the typical workflow from data generation over calibration development to routine use. This workflow is compliant to Pharmaceutical guidelines for NIR application‘s lifecycle.

Task	Lifecycle	NIRWare Operator	NIRWare Management Console	NIRCal
Setup reference application Set application to „approved“	●		●	
Record spectra of reference samples	●	●		
Define sample properties and values	●		●	
Calibrate Set calibration to „approved“	●			●
Copy application as template for routine use Define SOP	●		●	
Assign calibration to application Set application to „approved“	●		●	
Use for prediction / routine measurement	●	●		

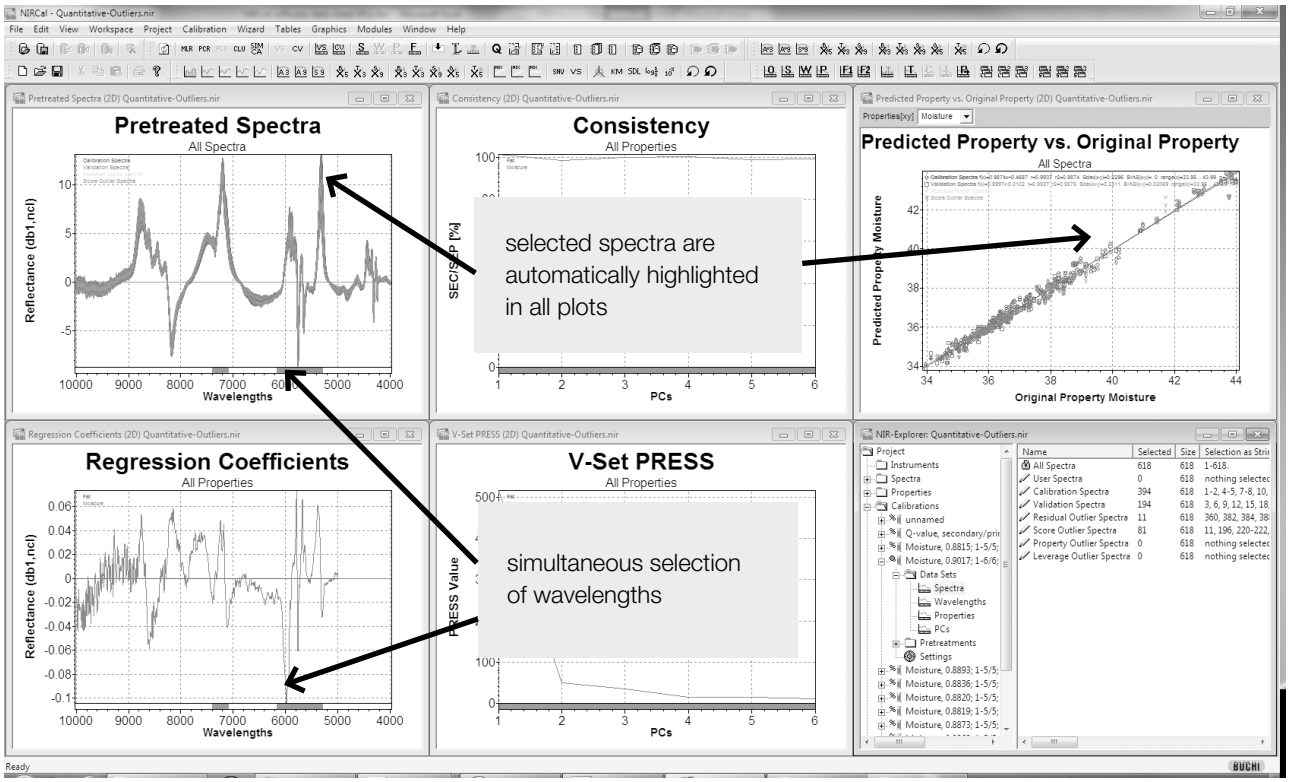
Description

Chemometrics

Multivariate quantitative and qualitative (classification, identification) calibration methods PLS, PCR, MLR, CLUSTER and SIMCA. Multivariate data analysis with PCA. Large selection of 45 data preprocessing algorithms (pretreatments) that can be used in any sequence, e. g. normalization, SNV, derivatives (1st/ 2nd/ 3rd), smoothing, transformations, offset correction, MSC, custom linear filtering.

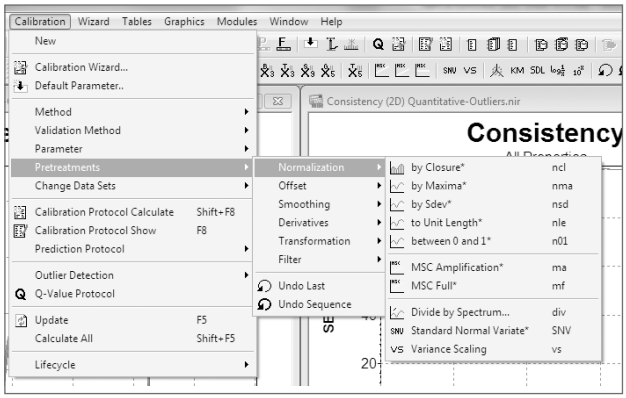
Data Visualization

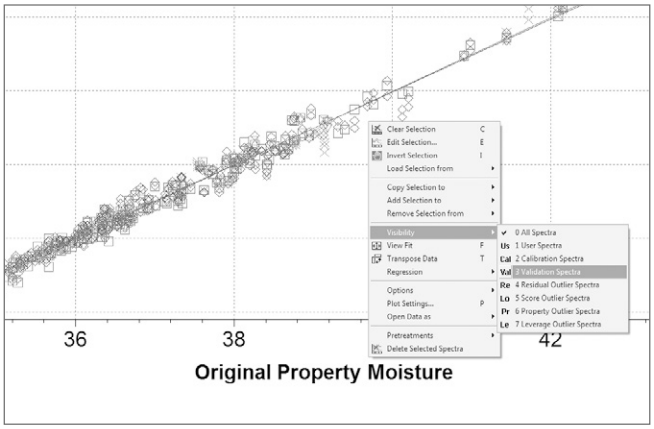
Interactive graphical visualization of spectral data, chemometric parameters and results in different plot types: line plot, parallel coordinates plot, scatter plot, surface plot in 1D, 2D and 3D. Interactive zooming, panning, scrolling, rotating, resizing, coloring, visibility and data info tooltips.



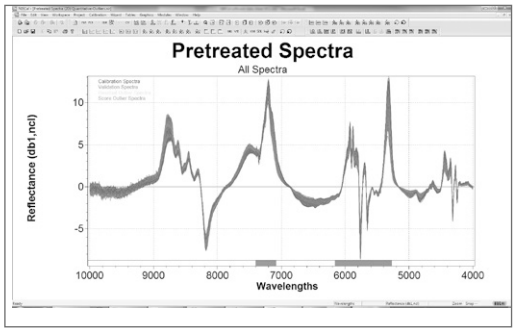
Easy selection of data sets (e.g. spectra, properties, wavelength, principal components) in graphic and table view. Live update of selected data within all corresponding plots and tables. Broad variety of visualization tools, like overview or dependency plots (e.g. data versus time, creator, instrument, property). Rapid calculations of large data sets.

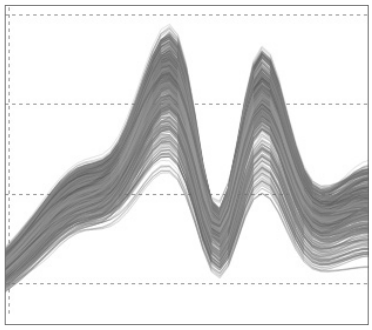
NIRCal provides context sensitive menus, customizable workspaces and toolbars.

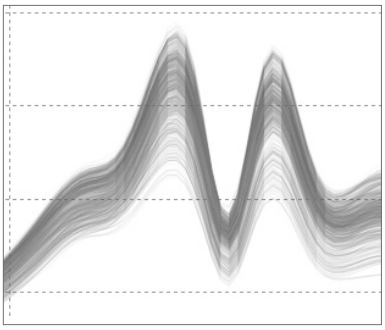




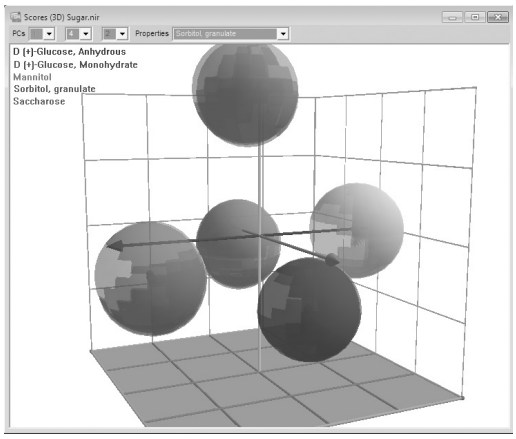
NIRCals graphical engine provides powerful visualization tools like anti-aliasing and alpha-blending.
Efficient review of big and complex data sets.





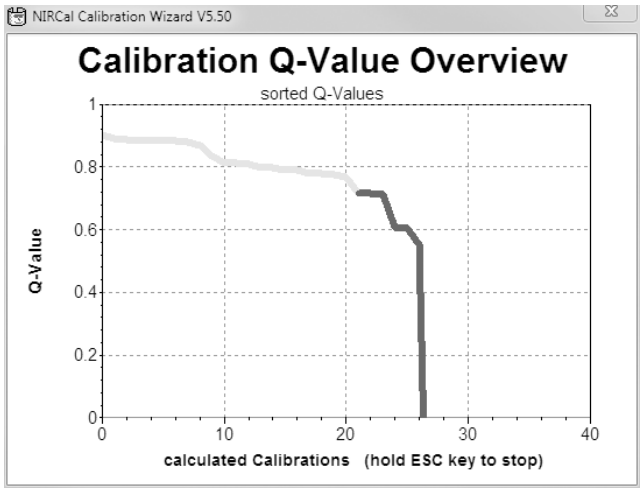


Interactive 3D views (free rotation, zoom, selection and more)
Example: Score plot to calibrate cluster models.

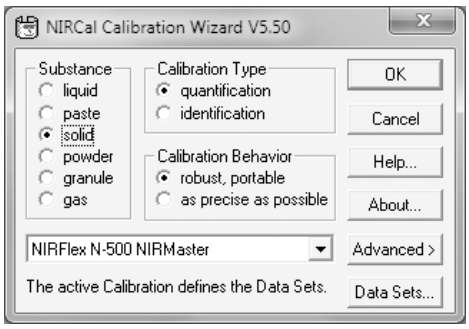


Calibration Wizard

Patented Calibration Wizard for automated calibration design based on BUCHI's long term application expertise.
Optimized results through automated outlier detection, selection of suitable algorithms and wavelengths, etc.

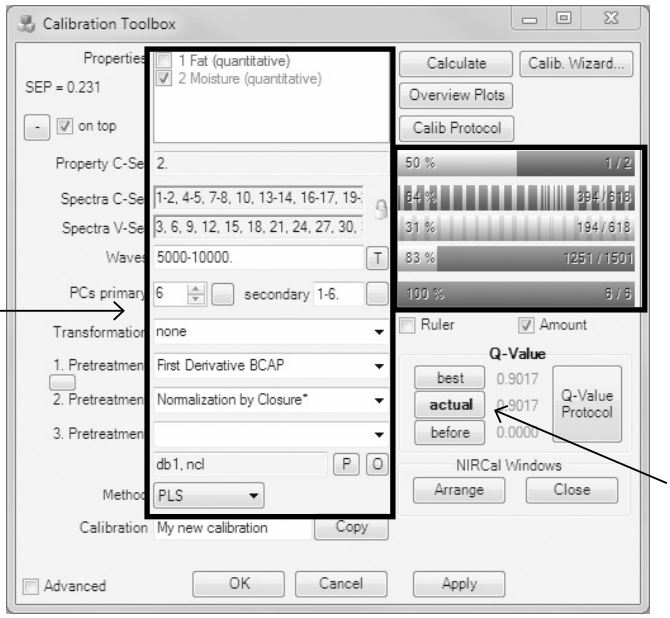


Wizard use requires just a few basic settings



NIRCal Toolbox

The NIRCal Toolbox is a compact cockpit view of the most relevant NIRCal calibration parameters enhancing method development productivity. NIRCal data views are automatically updated when calibrations are modified in the NIRCal toolbox.



Editable bar diagrams

All essential settings summarized and editable in one view

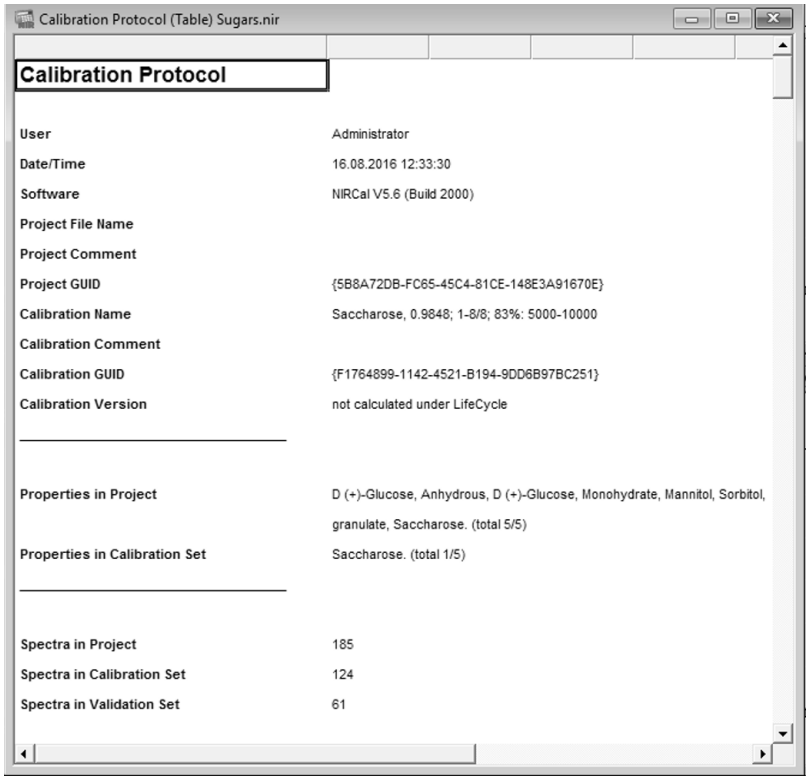
One-click switching allows immediate comparison of calibration versions

Data Exchange

NIRCal is compatible with a wide variety of data formats such as JCAMP-DX (jdx, dx), GRAMS (spc), MATLAB (dat), EXCEL (xls) and ASCII (csv)

Reporting and Method Validation Support

Detailed Calibration Protocol including settings, prediction results, outliers, used spectra, etc. Documented method verification and full traceability of changes and versions.



Calibration Protocol (Table) Sugars.nir

Calibration Protocol

User	Administrator
Date/Time	16.08.2016 12:33:30
Software	NIRCal V5.6 (Build 2000)
Project File Name	
Project Comment	
Project GUID	{5B8A72DB-FC65-45C4-81CE-148E3A91670E}
Calibration Name	Saccharose, 0.9848; 1-8/8; 83%: 5000-10000
Calibration Comment	
Calibration GUID	{F1764899-1142-4521-B194-9DD6B97BC251}
Calibration Version	not calculated under LifeCycle
Properties in Project	D (+)-Glucose, Anhydrous, D (+)-Glucose, Monohydrate, Mannitol, Sorbitol, granulate, Saccharose. (total 5/5)
Properties in Calibration Set	Saccharose. (total 1/5)
Spectra in Project	185
Spectra in Calibration Set	124
Spectra in Validation Set	61

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