

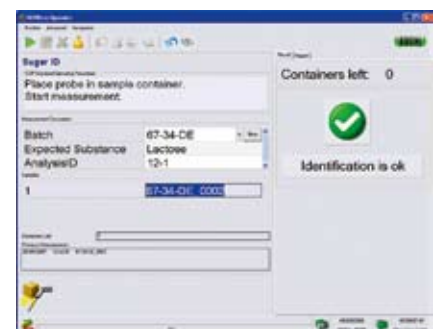
NIRWare 1.2

The NIRWare Software Suite, consisting of the NIRWare Operator and the NIRWare Management Console has been designed to meet all needs, from unregulated environments like food and feed industry and R&D laboratories to the highly regulated pharmaceutical production sites and QC laboratories. It allow creating, managing and using routine applications in an easy way thanks to the clear and user-friendly structure, provides access to all important data and is highly configurable to accommodate all specific requirements.



NIRWare Operator

The NIRWare Operator is the easy to use front end for data acquisition and routine measurements with easy to understand symbols and workflow. The integrated standard operating procedure guides users through the application. Only a few sample-specific entries are required to successfully run the NIRWare Operator.



- Highly configurable to support various routine procedures
- Access control with different User Levels
- Supported data input with Barcode reader including barcode splitting
- Input validation
- Quantitative result reporting with automatic average and standard deviation calculation, outlier detection and configurable action and warning limits
- Identification with At-line view using large fonts and result display (OK/Not OK), hitlists and outlier detection

- Content Uniformity Test Routine for tablets and capsules according to current USP/EP and JP

NIRWare Management Console

The NIRWare Management Console is the centralized tool that gives access to all configuration functions following a unique and logically structured design. It allows easy access to application and sample management as well as security settings and database maintenance, resulting in a rapid and efficient workflow.

- Access controlled, color coded snapins for easy navigation:

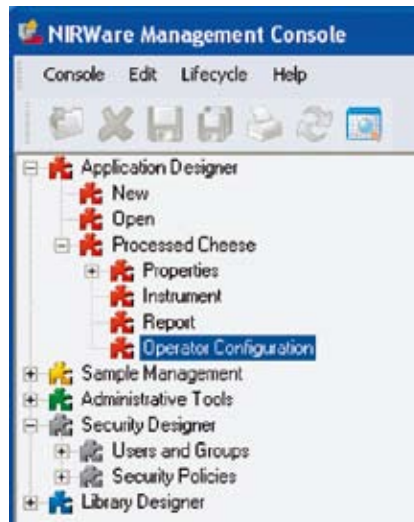
Application Designer: combines instrument parameter configuration, calibration and Operator settings for individual applications

Sample Manager: sample and reference value maintenance and result review

Administrative Tools: management of data exchange, database connections and database backup/restore

Security Designer: User and User Group Management and configuration of access rights

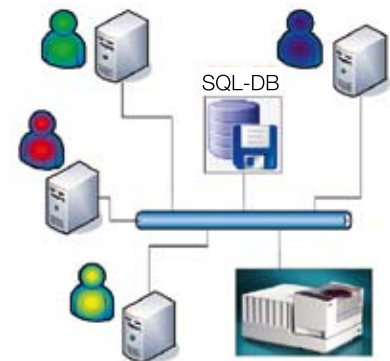
Library Designer: development of spectral libraries with hitlists for identification



- Standardized XML-data exchange between databases
- Reports with pdf and xls export function for external result archiving and data processing
- Filtering for data selection with storable filter templates
- Multilanguage capability (different asian and european languages supported)

Connectivity

- Database centric architecture using Microsoft SQL Server technology to ensure data security and traceability
- Stand-alone or centralized LAN installations



21 CFR Part 11 Compliance

- Full access control through highly configurable User Account Policy including:
 - Password history
 - Password complexity
 - Lockout mechanism in case of inactivity
 - Recognition of failed login attempts
- Configurable access control for individual software elements and applications
- Pre- and customer defined signature reasons for Electronic Signature
- Audit Trail
- Life Cycle based release- and version-management for applications

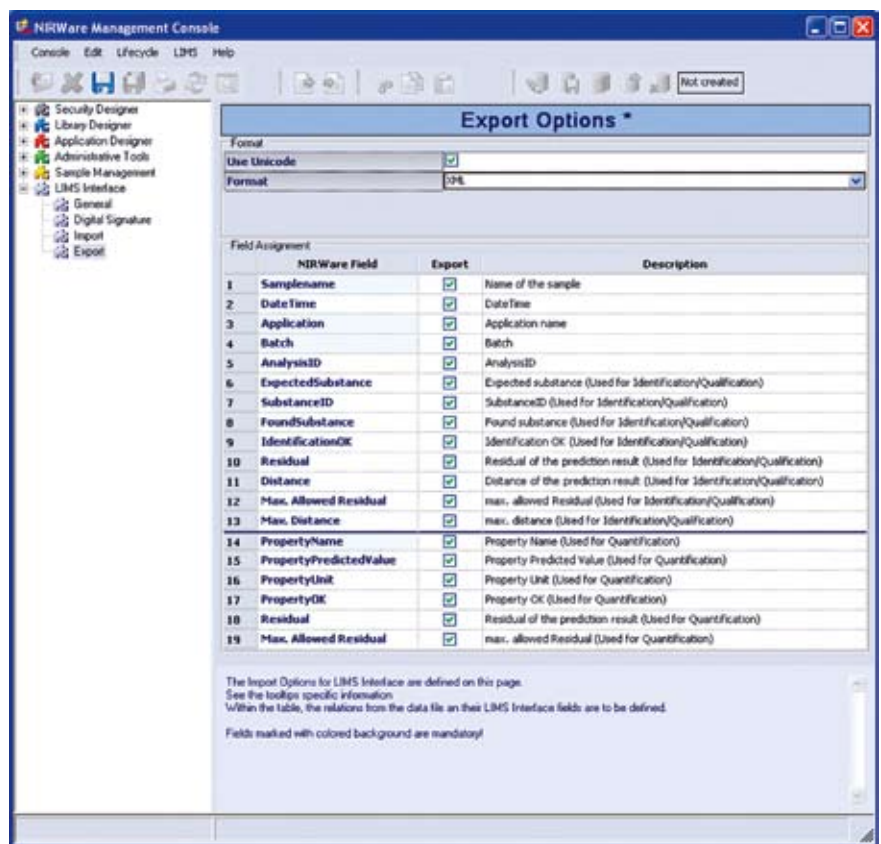
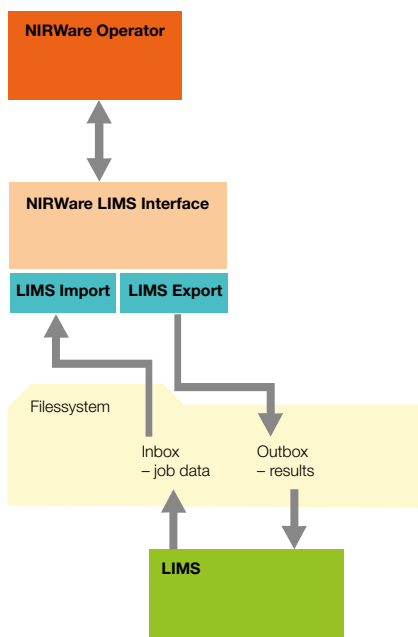
Control of Buchi NIRFlex N-500

- Automatic recognition of measurement cell type and add-on to ensure correct instrument configuration according to application requirements
- Hot swap of cells without system reboot
- Configurable periodic System Suitability Test (SST) routine and reference measurement
- NIRWare Advanced Diagnosis (NADIA) tool for extended system evaluation by service technicians
- Automatic test routine for USP Performance Verification (Optional)



NIRWare LIMS Interface 1.0

NIRWare LIMS Interface 1.0 – the link between the Buchi NIRWare Software Suite and LIMS (Laboratory Information Management System) or MES (Manufacturing Execution System). Direct job data import into NIRWare Operator and result export to the LIMS/MES software.



Secure

- Digital signature on exported files
- FDA 21 CFR Part 11 compliant environment

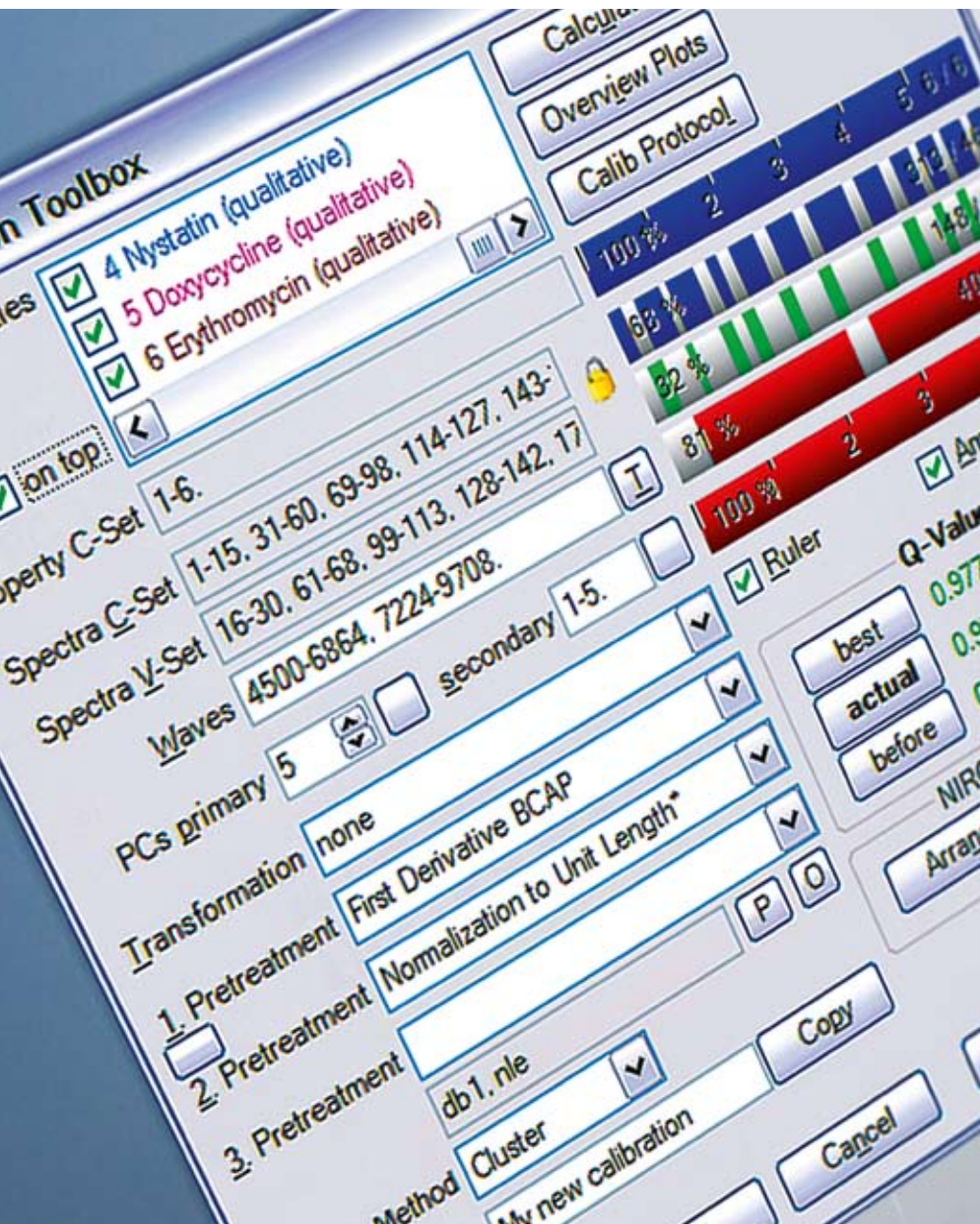
Flexible

- Support of XML and CSV file format for import and export
- Highly configurable file content

Easy

- Fully integrated add-on for NIRWare 1.2
- Configuration via NIRWare Management Console
- Single-click import of job data into NIRWare Operator

The Buchi NIRCal Chemometric Software has proven its value in practice for more than 10 years and is recognized by experts. Using the patented Calibration Wizard, even inexperienced users can easily develop robust calibrations. With NIRCal, calibrations for identity control and quantitative calibrations can be developed quickly and straightforwardly.



Key features

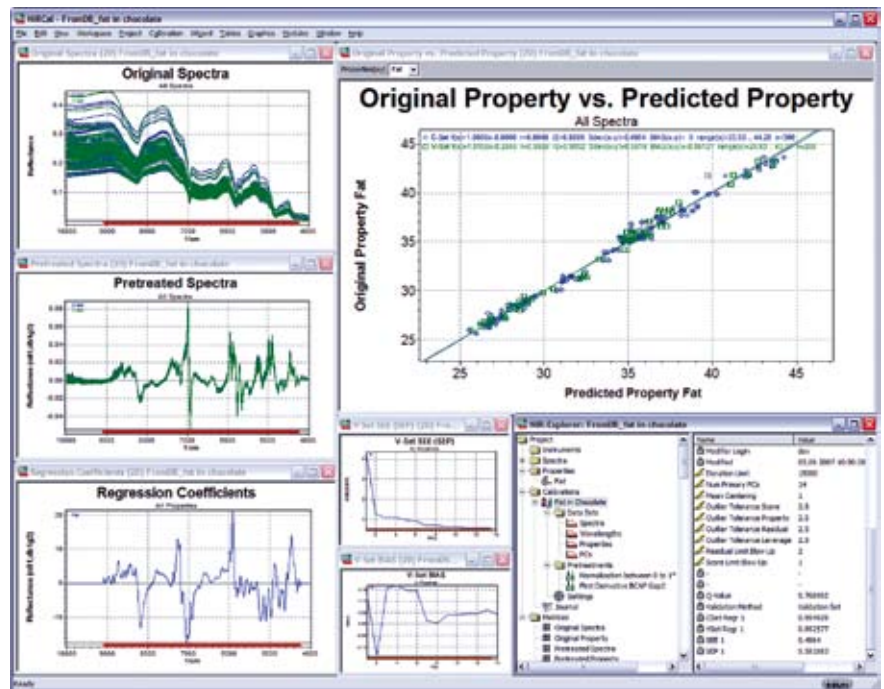
- Stand-alone Chemometric Software specifically developed for (NIR-) spectroscopic data. Works together with NIRWare 1.2
- Patented Calibration Wizard for automated knowledge-based calibration building
- Tree-based project data overview in NIR-Explorer (spectra, properties, calibrations, matrices)
- Database (SQL Server) or file based data handling
- Tracked Calibration development Life Cycle

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
- Arbitrary free wavelength (variable) selection possible (pretreatments depends on wavelength selection)



- Validation Set or Cross Validation with different grouping algorithms and jack-knifing
- Detailed Calibration Protocol including calibration version, all parameter settings, prediction results, used spectra
- Prediction protocols of selected external spectra to compare calibration performance and robustness
- Outlier Detection in modeling and prediction (Property, Residual, Leverage, Score)



Data Visualization

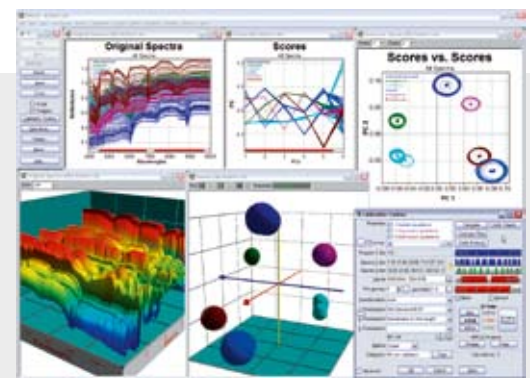
- Interactive graphical visualization of spectral data and chemometric parameters and results in different plot types (line plot, parallel coordinates plot, scatter plot, surface plot in 1D, 2D and 3D with zooming, panning, scrolling, rotating, resizing, coloring, visibility, data info tooltips). Immediately switching between wavenumber (cm^{-1}) and wavelength (nm).
- Easy selection of data sets (spectra, properties, wavelength, principal components) in graphics and tables
- Data link within all plots as well as tables
- Overview plots, Dependency plots (data versus time, creator, instrument, property)
- Fast calculation speed, graphics for large amount of data

Data Exchange

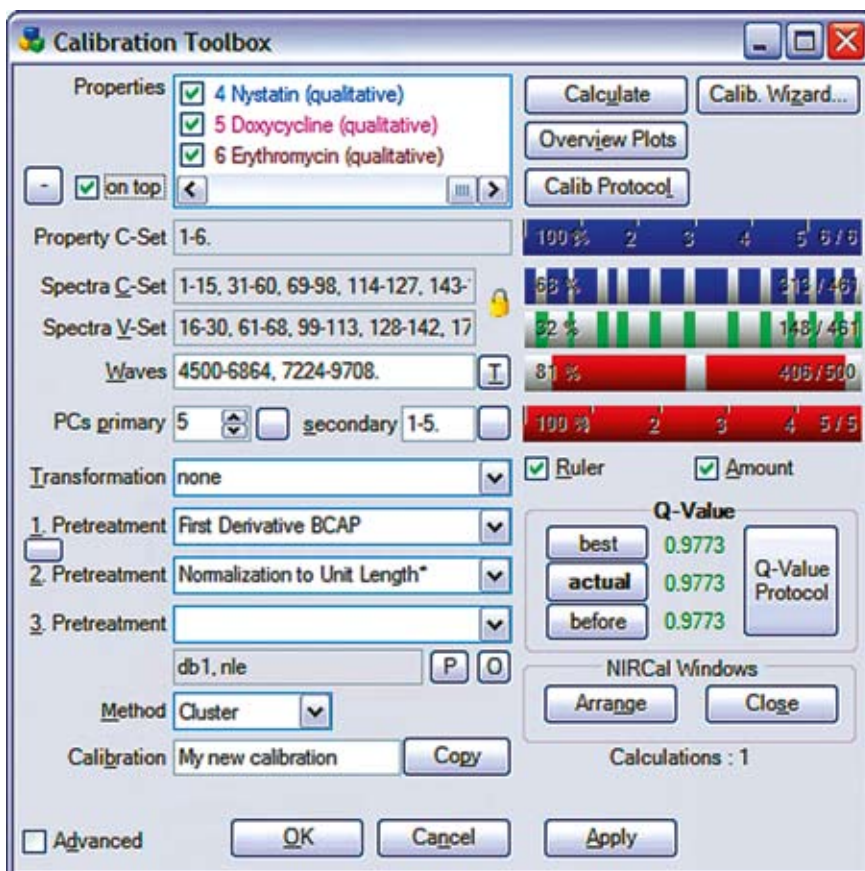
- Data exchange formats: JCAMP-DX (jdx, dx), GRAMS (spc), MATLAB (dat), EXCEL (xls), ASCII (csv)
- Cut and paste from tables and plots as Bitmap (bmp) or Windows Enhanced Metafile (emf)
- Spectra Converter to transfer NIRFlex N-400 spectra to the new NIRFlex N-500 spectral format

Customization

- Integrated BASIC macro programming environment to customize NIRCal directly or externally via COM interface to access the predictor, custom import/export, data conversion, data selection, calibration optimization



NIRCal Toolbox is a NIRCal add-on that provides quick and easy access to NIRCal calibration parameters and simplifies the calibration development. The intelligent and NIR focused GUI with Multilanguage support concentrates several NIRCal functions in one dialog. Interactive, visualized and easy-to-change pretreatments, swapping of the sequence order, and in-place exchange of algorithm types with immediate visualization of the effect. NIRCal Toolbox provides a fully featured information cockpit with all necessary parameters - all visible and directly accessible using the excellent NIRCal overview plots for quick judgement of the calibration result.



NIRCal Toolbox was created in order to

- Simplify calibration development
- Increase the productivity of calibration developers



NIR Solutions

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www.buchi.com Information Bulletin Number 49/2006

Cocaine and Heroin Content Determination with NIR

Confiscated street drug samples are mixtures with different drugs and cutting agents. Despite these different drug mixtures, exact NIR measurements are performed using the Buchi NIRFlex N-500 spectrometer. Visit www.buchi.com for more information.

NIRFlex N-500

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NIRFlex N-500 Solids Transmittance

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