

SensoLogic



The *SL* product family

A comprehensive software line for the daily practice of chemometric spectroscopy

Intelligent Spectroscopy...

Spectroscopy with chemometric data evaluation has been introduced with the Near Infrared Spectroscopy (NIRS) about 50 years ago. Today it is a mature technology which can replace conventional, mainly chemical analytical methods by much easier measurements with optical instruments. This becomes possible by modelling the relation between spectra and analytical results with proven mathematical/statistical methods.

Chemometric spectroscopy offers a non-destructive, clean and rapid determination of sample properties. In other words: when used in day-to-day routine analysis it helps to save time, resources and - above all - costs.

...with *SL*-Software Products

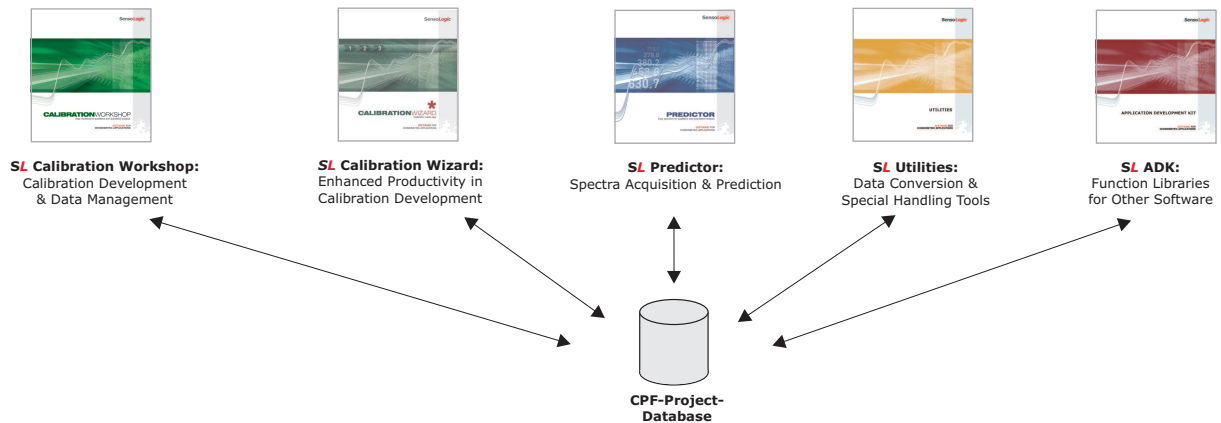
The combination of the various carefully balanced *SL* modules with a standardized project database structure meets the requirements for many areas of applications. *SL* Modules are used for tasks as different as:

- analyzing crop samples in agriculture,
- characterizing meat products in food production,
- determining parameters like the acid value of substances in the chemical industry,
- controlling octane numbers and other quality properties of gasoline in petrochemical refineries,
- identity and conformity testing through all stages - incoming material inspection, intermediate goods, and finished products.

The acquisition of spectra and reference analysis values, the subsequent development of individual calibration models and complete applications, and finally their employment in routine analysis - the entire workflow is supported in a practice oriented way. The software configuration can be adapted to the different requirements of each working environment and remains almost independent of the brand and type of instrument used.

Well-thought-out modularity and configuration settings make the *SL* family well suited for customizing and application-specific adjustment - wherever special requirements must be met but the development of individual software solutions is not economically justified.

The following **SL** - Modules are available:



SL Calibration Workshop:

For development and validation of spectroscopic analysis methods to determine quantitative and qualitative sample properties and for the database management of your projects

SL Calibration Wizard:

For very fast and easy creation of quantitative methods;
With step-by-step operator guidance, parallel processing of up to 50 calibration models and scalable automation capability this package becomes the ideal upgrade of SL Calibration Workshop for both beginners and experienced users.

SL Predictor:

For versatile routine application, at-line or in the laboratory, to perform spectroscopic data acquisition and evaluation with qualitative and quantitative models

SL Utilities:

A collection of helpful tools for the preparation of model development, data management and conversion

SL Application Development Kit

To use finished analytical methods and other content of SL project database files with software programs from third party suppliers or end users

SL Calibration Workshop 2.1

Modelling for quantitative and qualitative analysis and database management



Content:
Software **SL**
Calibration Workshop
Language: English
1 CD-ROM
1 Printed Software
Manual (English)

PC System-Requirements:
Intel- or AMD-Prozessor (> 1 GHz)
0,5 GB RAM
MS Windows
98/2000/NT/XP/Vista(32bit)/7(32bit)

The **SL** Calibration Workshop offers a selection of proven multivariate techniques for spectroscopic analysis. Complete applications can be configured which are ready to use for the prediction of unknown samples by the **SL** Predictor or other measuring software with **SL** ADK. All spectra, reference analysis data and models are clearly arranged and managed within a single database file which is the common basis for all other **SL** modules as well.

Functions of SL Calibration Workshop

Proven Multivariate Techniques

Methods of quantitative factor analysis:

- Principal Component Regression (PCR)
- Partial Least Squares Regression (PLSR)

Multiple Linear Regression (MLR) in wavelength space:

- Step-up Search (step-up/step-back method)
- Combination Search (complete permutation method)

The free combination of MLR and factor models with their particular outlier diagnostics enables results that are optimized separately for each predicted property.

Methods of qualitative factor analysis with Principal Component Analysis (PCA):

- Library Model (PCA discriminant analysis for groups)
- Cluster Model (PCA discriminant analysis for individual spectra)

File Import/Export

- JCAMP (*.dx, *.jdx)
- GRAMS Multifiles (*.spc)
- Unscrambler (*.una, *.uns)
- Sesame (*.spf)
- Binary files IDAS (*.dat)

Pre-treatment of Data

- Absorbance
- Moving average (Smoothing)
- First Derivative (two versions)
- Second Derivative (two versions)
- (0/1) Normalization
- Difference standardization (2 wavelength normalization)
- Whole Grain normalization (special case of difference standardization with wavelengths pre-selected for grain)
- Standard Normal Variate (SNV)

All algorithms can be combined in any order.

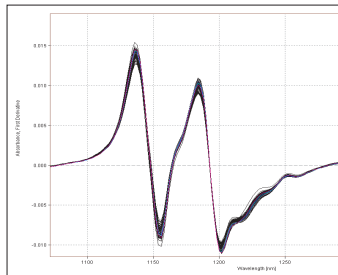


Fig. 1:
CH bands (2nd overtone) in a series of spectra of hydrocarbon mixtures, transformed with the first derivative of the absorbance values.

Filter Tools

- Selection of spectra depending on absorbance values at a selectable wavelength
- Selection of spectra depending on reference values of the assigned samples
- Removal of spectra depending on selectable outlier criteria
- Efficient search filters for database entries

Graphics Utilities

Several spectra, scatter and histogram plots for visualization and assessment of empirical data and models.

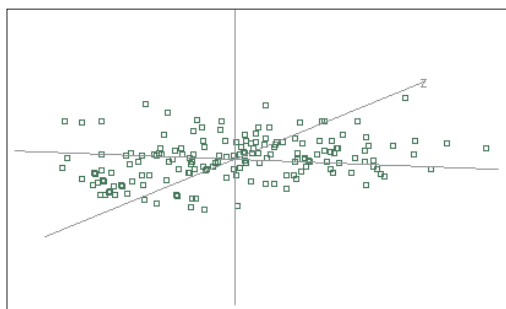
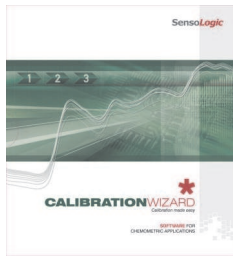


Fig. 2:
The scores plot of a spectra series can help to identify the existence of sub-groups or individual outliers.

SL Calibration Wizard 1.0

Rapid and easy modelling for quantitative analysis, with step-by-step guidance and extensive capability of automation



Content:
Software SL Calibration Wizard
Language: English
1 CD-ROM
1 Printed Software Manual
(English)

PC System-Requirements:
> 2 GB RAM
Screen resolution: mind. 1024x768
MS Windows 2000(.NET)/XP/Vista/7

SL Calibration Wizard is a true productivity-tool to be used side by side with the SL Calibration Workshop. Up to 50 calibration models can be developed in parallel using a workflow scheme with step-by-step guidance. With its well-arranged user interface, innovative functions and scalable automation this new program will be recognized as an indispensable member of the SL family by both beginners and experts.

Workflow of the SL Calibration Wizard

1. Selection of the working series and the sample properties to be modeled
2. Creation of test and calibration data sets
3. Selection of the transformations for spectra pre-treatment
4. Configuration of regression models
5. Computation of all models
6. Display of all calibration results
7. Configuration of prediction tests
8. Display of all test results
9. Validation of selected models
10. Summary of all results



Fig. 3: The SL Calibration Wizard clearly shows all relevant information and tools for the workflow step in process.

Features of SL Calibration Wizard Include

- Selection of transformation for spectra pre-treatment depending on variance and covariance analytical considerations
- Implementation of Detrend pre-treatment as polynomial regression
- Multivariate modelling with PLS-Regression and MLR Combination Search
- Significance test for comparison of alternative models
- Automated processing is individually configured for each wizard-step
- Automated outlier removal
- Prediction with estimated measurement uncertainty
- Significance tests for Bias and Skew
- User administration with storage of preferential settings for all steps

SL Predictor 1.6

Adaptable spectroscopy workbench for the daily routine analysis in lab or production



Content:

Software **SL** Predictor
Languages: English, German
1 CD-ROM
1 Printed Software Manual
(English, German)

PC System-Requirements:

> 1 GHz
0,5 GB RAM
MS Windows
98/2000/NT/XP/Vista/7

The **SL** Predictor provides a consistent user interface for spectra acquisition with instruments of different manufacturers and for evaluation with chemometric models (developed with **SL** Calibration Workshop or **SL** Calibration Wizard). With only a few inputs, the program is configured for the preferred data storage and output of results as well as for minimal operator interaction during the series of measurements for the sample batch.

Features of the **SL Predictor**

Configuration of the Work Station

- Spectrometers of different manufacturers are integrated by using their original drivers.
- For each instrument type the appropriate parameters are individually adjustable for spectra measurement and sample presentation options (e.g. rotating cups).
- The output formats for the measurement results via monitor, printer or file formats can be combined in a modular manner.

Main Screen in Measuring Mode

The user gets a clearly structured information including the current sample spectrum and - depending on the chosen application - the qualitative or quantitative analytical results. If in qualitative analysis a sample is not positively identified, the program lists a ranking of the most similar species available in the library. When quantitative methods are used, the individual measurement uncertainty can be assigned to each result.

Parameterization of the Measurement Mode

- Optional input of reference analysis values immediately with the spectra acquisition
- Spectra recording with or without direct saving to the SL-database series
- Spectra recording only or followed by qualitative or quantitative chemometric analysis
- Several scan-options like e.g. averaging of repeated measurements and graphical display of single spectra

Operational Safety

- User-administration with two access level (administrator and user)
- Multilingual user interface (English and German)

SL Utilities 2.0

A set of additional tools for the preparation of model development, data management and conversion



Content:
Software **SL Utilities**
Languages: English,
German
1 CD-ROM
1 Printed Software Manual
(English, German)

PC System-Requirements:
> 1 GHz)
0,5 GB RAM
MS Windows 98/2000/NT/XP/Vista/7

In addition to the import capability of the **SL Calibration Workshop** the **SL Utilities** offer special tools for file import to the database and conversion into the standardized, internationally accepted JCAMP exchange format.

Other utilities support the formation of representative subsets (Subset Selection) and the conversion of spectra (Wavelength Range Conversion).

The Database Viewer offers a quick overview of all entries of a project database file *.CPF (Chemometric Project File) and is especially useful for sorting and archiving purposes.

Database Viewer

Quick overview of the content of a CPF project file with explorer-like structure

- Sample with reference data
- Spectra, series and libraries
- Transformations
- Calibrations, methods and applications

Wavelength Range Conversion

Adaptation of spectra series to match other spectra abscissa:

- Truncation of the spectral range
- Interpolation to other increments or discret wavelengths
- Conversion between wavelength and wavenumber units

Subset Selection

Selection of a representative subset of spectra from an available series

- significance-based (Gauss-Jordan-procedure)
- random selection

SPC File Info, SPC File Import and ISI ASCII File Import

- Display the header-information of a selected SPC-file
- Batch import of GRAMS SPC single-files (with optional Excel-source for reference value assignment) into the CPF-database file
- Batch import of GRAMS SPC multi-files into the CPF database file
- Import of an ASCII-file, which has been created with WinISI-software (or earlier products of InfraSoft International), into the CPF database file

JCAMP Single-, CSV Single- and JCM Multifiles

can be converted by their respective conversion program into the standardized JCAMP multi-file format in order to import them into suitable other applications for further processing (e.g. SL Calibration Workshop).

SL Mini Soft Keyboard

This simplified display keyboard with large buttons can be installed independently and shall simplify the handling of touch-screen devices.

SL Application Development Kit 2.3

Versatile function libraries for your own software



Content:	PC System-Requirements:
Software <i>SL</i> Application Development Kit depending on licence typ	> 1 Ghz 0,5 GB RAM MS Windows 98/2000/NT/XP/Vista/7
1 CD-ROM	

The *SL* Application Development Kit consists of several function libraries (*.dll), which can be used to create a new integrated software application on the *SL* platform. Software engineers can get a developer license package which contains PDF documents in English for each library as well as a Visual Basic demo program. A corresponding runtime license for each target system can also be offered as a partial license if only quantitative or only qualitative methods are used by the application.

Functions of *SL* Application Development Kit

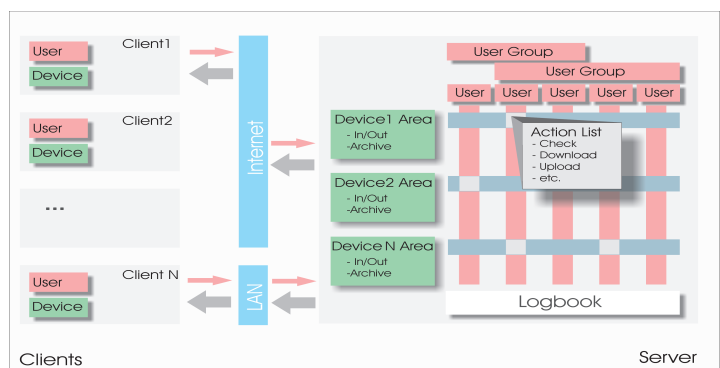
- Quantitative prediction with MLR and factor regression models including their respective outlier-detection
- Qualitative prediction with PCA library and cluster models
- Direct write and read access to spectra series and other database entries
- Special functions for the standardization of spectrometers
- All transformation algorithms of *SL* Calibration Workshop and *SL* Calibration Wizard for pre-treatment of spectra
- Additional functions for integration in Visual Basic and LabView applications

SL Calibration Network

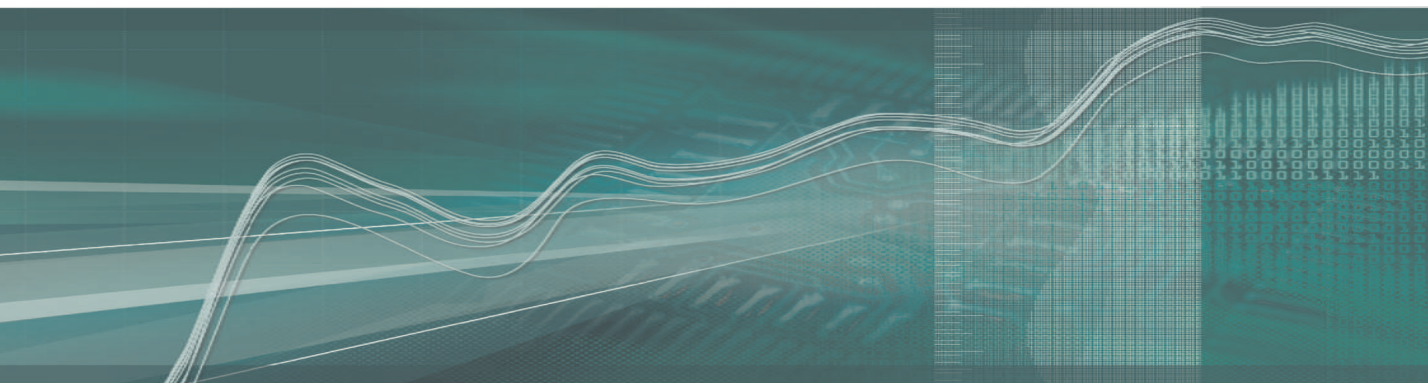
Calibration network for spectroscopic analytics

Performance Features:

- Data transfer via LAN or Internet
- User and access administration
- Transmission of spectra and reference data
- Transmission of calibration models
- Scalable for different networks
- Instruments and software from different manufacturers can be integrated



On request we are pleased to suggest you a special solution for your organization.



Calibration Development

To our customers, we offer calibration services ranging from the development of a single calibration to long-term support for particular analytical methods, and to full-service calibration development and maintenance. For further details, please see our separate info material on SL Training and Calibration Services and the product information SL Calibration Network.

Partners

In order to ensure problem-free operation with all *SL* products for our customers, we cooperate closely with the manufacturers of spectrophotometers who agree to our use of their original instrument drivers and/or who use the *SL* Application Development Kit in their software.

On request you can get our *SL* Partner List where you will find the manufacturers and distributors who support the *SL* platform in combination with their products. As we are preparing to implement more drivers, we would also like to discuss with you the chance of implementation of your preferred instrument.

Training Courses

SensoLogic offers training courses for groups or companies as an introduction to the most efficient use of *SL* products and to the spectroscopic and chemometric principles on which they are based. For further details please see our Brochure on *SL* Training and Calibration Services. Announcements of training courses are periodically published on our website (www.sensologic.com).

Price List

To obtain our current price list for the modules of the *SL* product family, please send your request to info@sensologic.com (subject: *SL* price list).

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