

## 1 Purpose

This document describes the fixed bugs as well as improvements in the following new software version in comparison with the previous version.

- New version: 4.2.100
- Old version: 4.1.11

## 2 New features

Topic	Description
ModelExpert	Automated model parameter determination.  Available under <b>Training Sets ► [Example Training Set] ► Overview.</b>
SmartSync	Automatic and configurable sample organization.  Available under <b>Compliance ► Compliance Configuration ► General ► Synchronization Settings.</b>
Data retention period	FDA 21 CFR Part 11 only requires that data is kept for a certain amount of time: This feature allows the user to determine a retention period. Also, it is possible to keep data forever. Defaults are 5 years.  A review and backup are required before removing expired data.  Available under <b>Compliance ► Compliance Configuration ► General ► Data Retention.</b>
Validation	Built-in validation sets and ROC curves to validate a model and test all parameters for the best possible performance.  Available within each training set.

Topic	Description
IT Admin user level	<p>A limited user level that has permissions to change IT-type settings but not to modify or generate new data.</p> <p>Permissions include:</p> <ul style="list-style-type: none"> <li>▪ Manage database (location, backups...)</li> <li>▪ Manage users/passwords</li> <li>▪ Manage software configuration (logout time, synchronization settings, custom reports, data export...)</li> </ul> <p>Available as a user level in the <b>User Management</b> window.</p>
Group Viewer	<p>A new tool to group spectra and view them together with the same color. This feature is useful for comparing different vendors, containers, batches etc.</p> <p>Available in the <b>Sample</b> window.</p>
Average spectra	<p>A fully traceable average function with no loss of information.</p> <p>Available in the ribbon and in the context menu of the <b>Sample</b> browser.</p>
Masks/Regions	<p>Set regions for a training set where the model will focus. Allows the user to ignore portions of a spectrum for specific classification.</p>
Custom signature reasons	<p>Modify or remove existing signature reasons. Add new signature reasons.</p> <p>Available under <b>Compliance ► Compliance Configuration General ► Signature Settings</b>.</p>
Configuration settings with export/import	<p>Deploy the same configuration on multiple computers.</p> <p>Available under <b>Compliance ► Compliance Configuration</b>.</p>
Library confusion matrix	<p>Test every library entry against the rest of the library to check for similarities. Output ranges from simple list sorted by correlation score to full Excel color-coded spreadsheet.</p> <p>Available within each library.</p>
Combine libraries function	<p>This feature gives the user the ability to merge multiple libraries. This feature maintains the original library and adds a new one.</p> <p>Available after selecting multiple libraries in the <b>Libraries</b> window.</p>

### 3 Improvements

Topic	Description
P-value available in columns	<p>Making the verification p-value available as a list item in the <b>Sample</b> browser.</p> <p>Available in the context menu in the <b>Sample</b> browser.</p>
Remove empty folders	<p>Remove empty folders in the Sample tree.</p> <p>Available in the context menu in the Sample tree.</p>
Additional model preprocessing options	<p>Improvements to the PCA modeling by enabling more preprocessing options.</p> <p>Available within each training set.</p>
Preview spectra after preprocessing	<p>New option to preview training set and validation set spectra with all preprocessing applied.</p> <p>Available within each training set.</p>
Additional metadata	<p>New metadata fields are now available:</p> <ul style="list-style-type: none"> <li>▪ Supplier</li> <li>▪ Product ID</li> </ul> <p>Available in the info of each test.</p>
Model plots colored by metadata	<p>When reviewing PCA plots, tests can be colored by specific metadata fields. This helps in model analysis.</p> <p>Available within each training set.</p>
Audit Trail search field size	<p>Increased search field size to handle full GUIDs without clipping.</p>
Copy GUID to clipboard	<p>New button to copy object GUID to clipboard. This allows the user to search the audit trail by GUID.</p> <p>Available in the info for each object.</p>
Copy certain objects	<p>Ability to duplicate operating procedures, training sets and libraries.</p>
Built-in checks for library and training set building	<p>Runs a check when samples are added to training sets and libraries. Training sets expect similar spectra while Libraries expect dissimilar spectra. This feature prevents incorrect data in training sets and duplicate entries in libraries.</p>
Local time format	<p>This gives the user the ability to see the dates and times in the same format as the date and time on the computer (e.g. DD/MM/YYYY vs. MM/DD/YY).</p> <p>Available under <b>Compliance ► Compliance Configuration ► General</b>.</p>

Topic	Description
Default smoothing parameters	Changed default smoothing parameters to more useful defaults.
Database information panel	<p>This new panel shows statistics about the database including:</p> <ul style="list-style-type: none"> <li>▪ Number of samples, operating procedures, training sets, libraries</li> <li>▪ Size of database</li> <li>▪ Location</li> </ul> <p>Available under <b>File ► Advanced ► Info</b>.</p>
Database reset option	<p>The database reset function gives the administrator the option to clear a database without losing users, operating procedures, training sets, libraries of the entire compliance configuration. The audit trail remains intact except for the sample-related events.</p> <p>Available under <b>File ► Advanced ► Database ► Reset</b>.</p>

#### 4 Fixed bugs

Topic	Description
System suitability test global status	Fixed behavior when Polystyrene verification failed but all other parts passed.
Empty folder options	Cleaned up empty folder behavior and options

#### 5 Known issues

None.

#### 6 Compliance

The new software version has been certified by a third party for compliance with 21 CFR Part 11 and GAMP.