

What's new in dbLabCal V3?

Update dbLabCal V3 SP7-> dbLabCal V3 SP8

(February 2016)

New

1. Data Import from MSD Instruments

2. ICP-MS Import

Either "MEAS. INTENS. MEAN" or "NET INTENS. MEAN" data will be imported into dbLabCal from the "*.rep" File depending on which column is found most left.

So far "MEAS. INTENS. MEAN" only where imported.

3. Result export according new BI's DTA

Sponsor specific export format updated.

4. User can select also "comments to chromatogram" in the Subject result table

Options Subject Sample Results

Columns

Dilution Factor

Sequences

Of Used Chromatograms Only

Of All Chromatograms

Comment

to result

to chromatogramm

Show LOQ and 10xLOQ

RandRep Ok Cancel

5. Also ReadOnly users have access to export menus.

6. dbLabCal V3 SP8 is Windows 8.x and Windows 10 compatible

7. Reassay and Incurred Samples Reporting Options modified

2 „exotic“ and never used ways of ISR calculations were removed since meanwhile, the ISR evaluation is performed in general according to the „FDA“ Method

Acceptance criterion of which part of ISR must have difference between the both results less than 20% is set to 2/3 and not editable

Options Reassays

Rules for reported Result (Reassays)

dbLabCal default (mean if diff.<=28%*), total 2 or 3 assays

1st accepted result (total 2 to 9 assays)

Lang & Bolton Rule (median/mw, <15% / <30%, total 2 or 3 assays)

HoLaRo Rule (mean if diff.<=28%*), total 2 or 3 assays

Max. deviation between re-assays in [%] of mean: conc.>lowest QC 28 10-40%

conc.<=lowest QC 28 10-60%

Rules dev% calculation (Incurred Samples)

FDA: diff. between ISR and FIRST in % of mean dev% = (ISR-A) / mean(ISR+A)

EBF: diff. between ISR and FIRST in % of FIRST dev% = (ISR-A) / A

Max. difference between Incurred Samples in [%] 20.0 10-40%

Action all peaks

Reset all choices!

Do auto choice, do not overwrite already set values!

Do auto choice for all reassays! Overwrite already set values!

Sort reassays according to batch number (default sorting is according batch start date)

Ok Cancel

What's new in dbLabCal V3?

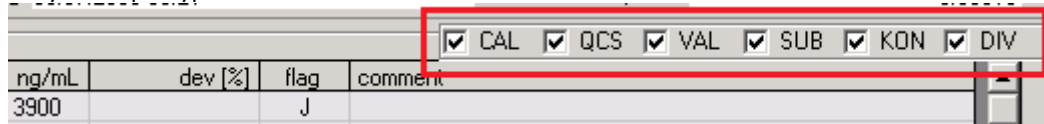
UI (user interface) improvements

8. Significant figures also selectable after right mouse click


So far the significant figures could be changed through the Project/Options menu only

9. Batch Sample Type Filter

Grey if sample type does not exist in batch



10. Alternative Analyte and Batch Navigation

Through mouse click on left/right arrows 

11. Tables scrolling using mouse wheel possible

12. ASCII export format adapted (no comments)

Bug fixes

- HLR Export Date Bug
- Quad.Regr. Overflow Bug
- ELISA 1# Bug
- ELISA Min.Max. Bug
- Create new user while project archived Bug
- ASCII export when only 1 NOR value Bug

What's new in dbLabCal V3?

Update dbLabCal V3 SP6-> dbLabCal V3 SP7

(June 2011)

1. Batch Status "locked", S and E flags in "locked" batches

PBI can lock a batch after it was previously accepted (batch status set to "accepted"). Consequently, even PBI cannot (accidentally) change sample name or sample flag in an accepted batch.

Furthermore, automatic procedure started in the Acceptance Criteria Dialog to set flags (set internal standard response flag (S) or exclude Standard or QC sample (E) will ignore samples in locked batches.

	Standards	QC's
Max. deviation from nom. conc. at LOQ / LQC	20 %	15 %
Max. deviation from nom. conc. (remaining CALs/QCs)	15 %	15 %
Min. number of used and accepted values	6	4
Coefficient of determination (R ²) value	0.98	1 ?
Max. accepted intercept in % LOQ	50	
Set flag for QCs/VALs to E if deviation higher than	off %	
Set flag for SUBs to S if IS not within mean(*) ±	off %	S
Set flag for QCS to S if IS not within mean(*) ±	off %	S

(*) = CAL
 CAL+QCS

? At least 1 QCs at the same concentration must fit acceptance criterion!

All project's batches are "locked" automatically after project data were released (project status set to "released").

Also all project settings are locked if at least one batch has status "locked".

2. Chromera Import

Data import from HPLC-ICP-MS instrument controlled by Chromera software is possible.

3. HoLaRo non barcoded export

Results export according HoLaRo's non-barcoded specifications is possible.

4. System Audit Trail

System Audit Trail (menu db->System AuditTrail) tracks and shows all system changes (user creation, changes of permissions/roles, changes of database options etc.)

5. Improvements: LC-MS/MS Data Import, Analyst Software (AB SCIEX) (ISR tag, Chromatogram Flag, Annotations and Comments)

Sample is marked as ISR automatically during data import from Analyst if the user has written the text „ISR“ or “incurred sample...” already in Analysts result table Sample Annotation column.

Chromatogram flags and comments are automatically set during data import from Analyst if the user has written the flag and comment already in Analysts result table Analyte Annotation column.

Syntax is: FLAG <comma or space> comment

Exaple: “N, interference”

“N, instrument failure”

“X, instrument failure, reinjectet”

“D, sample destroyed”

dbLabCal writes a filename.lca.ok file after succesfull import of an lca file. The lca.ok file is used in the program AnalystDataCheck to document the dbLabCal data import. This information is part of the chromatography data flow definition if the Analyst raw data is “full electronic data” and not paper.

6. Improvements: Incurred Samples Reporting

It is possible to toggle the ISR tag (pressing CTRL-R) also directly in the Reassay and/or Incurred Samples Result view

The difference between the incurred samples assays is expressed with sign (formerly as absolute difference)

In case of having reassayed a sample (with 2 or more analytes) due to „standard reassay reason” as well as an ISR sample, the results are presented for all analytes in both result tables (Standard reassays and Incurred Samples)

7. Reference mean for IS batch acceptance based on “only” CAL mean or based on mean of all CAL and QCS samples possible

	Standards	QCs
Max. deviation from nom. conc. at LOQ / LQC	20 %	15 %
Max. deviation from nom. conc. (remaining CALs/QCs)	15 %	15 %
Min. number of used and accepted values	6	4
Coefficient of determination (R ²) value	0.98	1
Max. accepted intercept in % LOQ	50	

Set flag for QCs/VALs to E if deviation higher than	off %	
Set flag for SUBs to S if IS not within mean(*) ±	off %	S
Set flag for QCS to S if IS not within mean(*) ±	off %	S

(*) = CAL CAL+QCS

8. Project Load with "full text search"

Additional filter in Load Project dialog allows user to find projects by any text in all project codes, comment, analyte name or matrix.

Project	Comment	Project Type	changed	Sponsor Code	GLP-Code
KA001	5-ASA/N-Acetyl-5-ASA in Plasma and Urine	Routine	26.04.2000	CRO-PK-99-22	BA
KA018	5-ASA/N-Acetyl-5-ASA in Plasma and Urine	Routine	09.08.2000	CRO-00-15	BA
LA131	5-ASA/Ac-5-ASA	Routine	10.10.2001		BA
TX021	5-ASA/Ac-5-ASA in Humanplasma	Validation	16.07.2009		BA

Analyte	Matrix	Status	Method	Project Type	Filter																											
					<table border="1"> <tr> <td>all</td> <td>all</td> <td>all</td> </tr> <tr> <td>last week</td> <td>Routine</td> <td>GLP only</td> </tr> <tr> <td>last month</td> <td>Validation</td> <td>non-GLP only</td> </tr> </table> <table border="1"> <tr> <td>all</td> <td>all</td> <td></td> </tr> <tr> <td>defined</td> <td>QC in-progress</td> <td></td> </tr> <tr> <td>started</td> <td>QC-ed</td> <td></td> </tr> <tr> <td>finished</td> <td>QA-ed</td> <td>asa/</td> </tr> <tr> <td>data released</td> <td></td> <td></td> </tr> <tr> <td>archived</td> <td></td> <td></td> </tr> </table>	all	all	all	last week	Routine	GLP only	last month	Validation	non-GLP only	all	all		defined	QC in-progress		started	QC-ed		finished	QA-ed	asa/	data released			archived		
all	all	all																														
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data released																																
archived																																

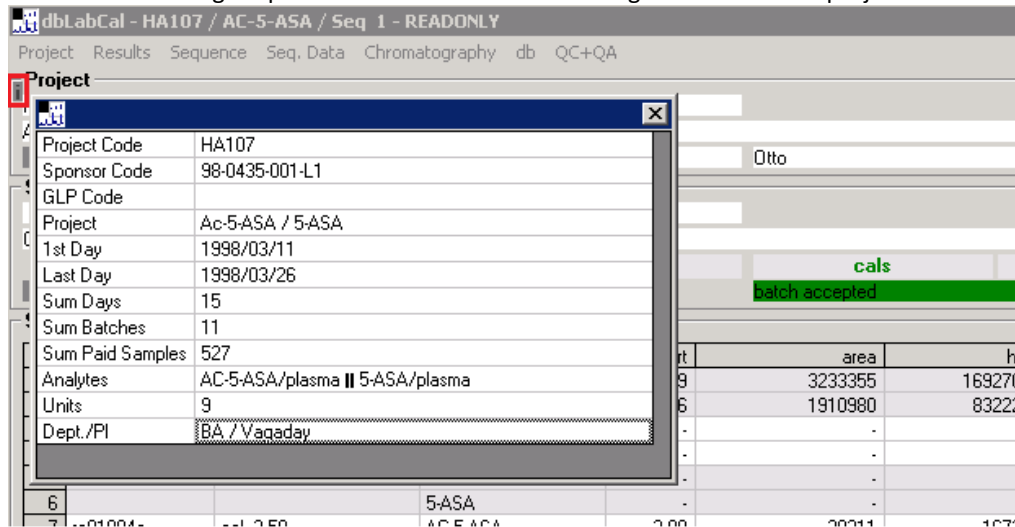
9. Batch Sample Type Filter

Formerly, batch sample type filter was opened by clicking on the „name “column in the batch view. Now, the filter is always visible on the right upper corner. It allows reducing the batch view to the selected sample type(s).

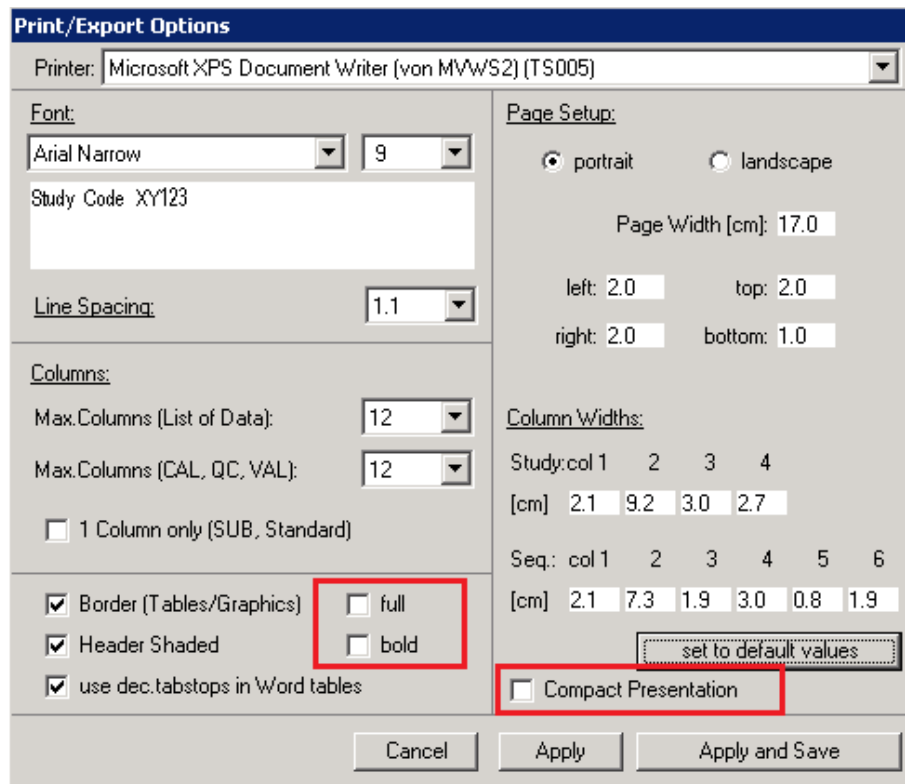
ng/mL	dev [%]	flag	comment
3900		J	
3780		J	

10. Project Info Display

An additional dialog is opened after click on the  showing some additional project information.



11. More Options in Word Export



Full borders, Header line with font bold and Compact presentation (Export only)

12. Force QC-Check

Export to ASCII file allowed only after the QC check was completed. (PBI's "extra wish key" is possible.)

13. Load Project as „Read Only“

ReadOnly user has by default read access to all dbLabCal projects. Now, also analysts and PBIs can open any projects with “readonly” permission while pressing the CTRL key if opening the Load Project dialog.

Load Project - READONLY

Project	Comment	Project Type	changed	Sponsor Code	GLP-Code
KA001	5-ASA/N-Acetyl-5-ASA in Plasma and Urine	Routine	26.04.2000	CRO-PK-99-22	BA
KA018	5-ASA/N-Acetyl-5-ASA in Plasma and Urine	Routine	09.08.2000	CRO-00-15	BA
LA131	5-ASA/Ac-5-ASA	Routine	10.10.2001		BA
TX021	5-ASA/Ac-5-ASA in Humanplasma	Validation	16.07.2009		BA

Analyte	Matrix	Status	Method	Project Type	Filter
Ac-5-ASA	Plasma	data released	HPLC-FL	Validation	all
5-ASA	Plasma	data released	HPLC-FL	Validation	last week last month

Filter	Filter
all	all
defined	QC in-progress
started	QC-ed
finished	QA-ed
data released	
archived	

Cancel Ok

Program bar shows, if the user has opened a project as read only user.

dbLabCal - HA107 / AC-5-ASA / Seq - READONLY

Project Results Sequence Seq. Data Chromatography db QC+QA

Project
 HA107 98-0435-001-L1
 Ac-5-ASA / 5-ASA
 memo BA Vagaday Otto

Sequence
 1 9 Otto
 CAL 01 - Revalidierung (Intra Day + LLQ)
 memo Acceptance cals
 batch accepted

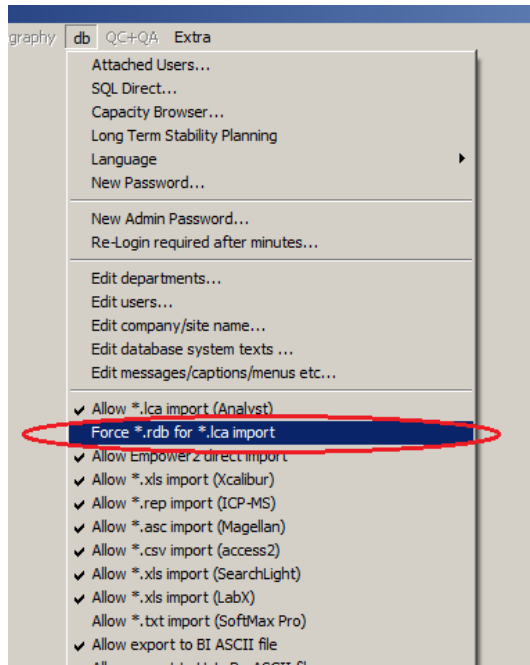
Sequence List

	file/sampleID	name	analyte	rt	area	hi
1	ro01001a	sss	AC-5-ASA	3.09	3233355	169270
2			5-ASA	5.36	1910980	83222
3	ro01002a	w.b.	AC-5-ASA	-	-	-
4			5-ASA	-	-	-
5	ro01003a	Blank	AC-5-ASA	-	-	-
6			5-ASA	-	-	-
7	ro01004a	cal 2.50	AC-5-ASA	3.09	28211	1673
8		cal 1.00	5-ASA	5.37	14575	754
9	ro01005a	cal 6.25	AC-5-ASA	3.15	82562	4268

14. dbLabCal Analyst Data Import Check

If the Administrator activates the function (see below), dbLabCal will:

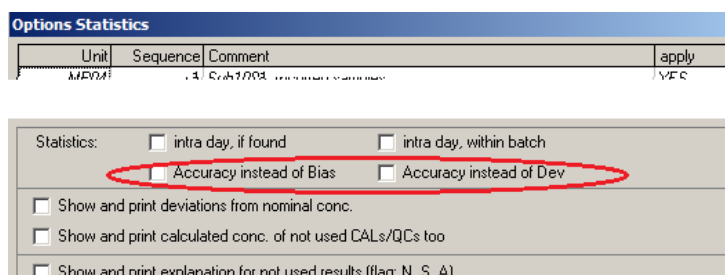
- expect the lca-file be in the same folder with the respective Analyst's rdb-file having the same file name (e.g.: batch001.rdb - batch001.lca, batch002.rdb - batch002.lca etc.)
- lock the Analyst's rdb-file in that no data can be changed (chromatograms re-integrated) after the rdb-file data were imported into dbLabCal



15. New Options in Option Statistics Dialog

Accuracy instead of % bias or % dev possible.

(e.g.: bias=1.23% - accuracy=101.23%, bias=-1.23% - accuracy=98.77%)



16. More options for Incurred Samples Reporting

ISR is possible according FDA, EBF (European Bioanalytical Forum) guidelines and recommendations and also according two more (slightly different) options.

- Diff. of ISR and first measurement in % of mean (=according FDA)
- Diff. of ISR and first measurement in % of first measurement (=according EBF)
- Diff. of ISR and first measurement in % of final(reported) result (some clients)
- Diff. of ISR and first measurement in % of mean of final and ISR (some other clients)

Options Reassays

Rules

- dbLabCal default (mean if diff.<=20% %), total 2 or 3 assays)
- 1st accepted result (total 2 to 9 assays)
- Lang & Bolton Rule (median/mw, <15% / <30%, total 2 or 3 assays)
- HoLaRo Rule (mean if diff.<=20% %), total 2 or 3 assays)

Max. difference [%] for mean value: 10-40%

Rules (Incurred Samples)

- FDA: diff. between ISR and FIRST in % of mean dev% = (ISR-A) / mean(ISR+A)
- EBF: diff. between ISR and FIRST in % of FIRST dev% = (ISR-A) / A
- calc. diff. between ISR and FINAL in % of FINAL dev% = (ISR-F) / F
- calc. diff. between ISR and FINAL in % of mean dev% = (ISR-F) / mean(ISR+F)

Max. difference between Incurred Samples in [%] 10-40%

accepted Incurred Samples at least 66.7-100%

Action

- Reset all choices!
- Do auto choice, do not overwrite already set values!
- Do auto choice for all reassays! Overwrite already set values!

Show last chromatogram flag as:

- Sort reassays according to batch number (default sorting is according batch start date)

Cancel Ok

17. ISR Usage in Standard Re-assays not Allowed by Default

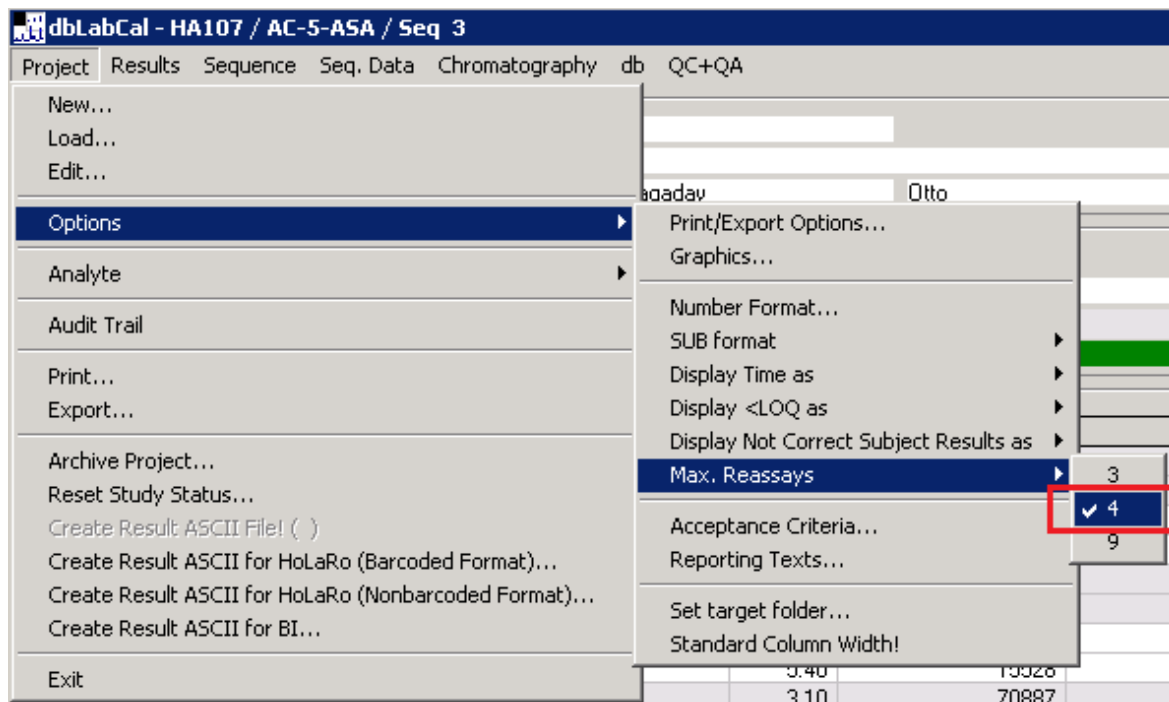
In case a sample had to be re-assayed because of ISR and also because of “standard re-assay reason” like bad chromatography etc., it is now by default not possible to choose final/reported value using the ISR. But, with CTRL key at right mouse click while selecting the final result allows the PBI to use the ISR, anyway. (=PBI’s “extra wish key”)

ISR are displayed in brown color for easier identification.

What's new in dbLabCal V3?

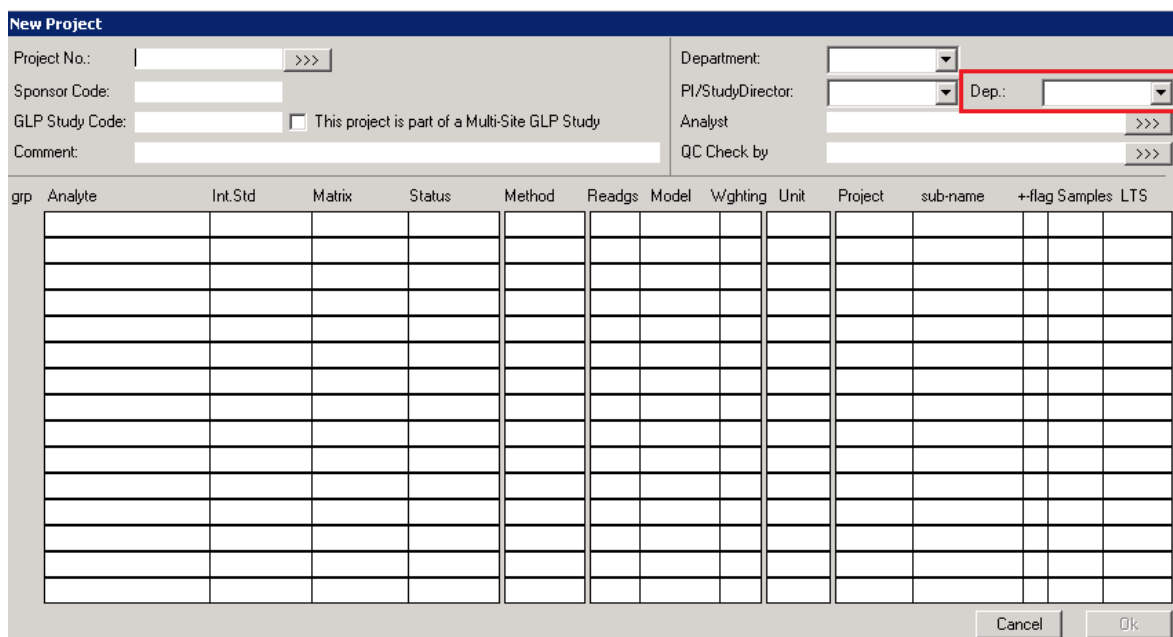
18. Full 4 Re-Assay Reporting

It is possible to report any value and any “mean value combination” also having 4 re-assays. So far the limit was 3 reassays.



This option is set through the menu Project->Options->Max.Reassays. Previously it was located in the “New Project” / “Edit Project” dialog.

19. Deputy PBI



Deputy of the PBI (with PBI's projects permissions) can be assigned to a project.

+ small bug fixes

Update dbLabCal V3 SP5-> dbLabCal V3 SP6

(October 2009)

1. dbLabCal imports Data from Searchlight and Empower2

Data import from another IA instrument possible.

„Direct import from Millennium“ adapted for Empower2.

2. „Working Range“ for CALs

Working Range (in addition to LOQ, ULQ) can be defined in IA projects. Chromatogram flags will be set automatically for results outside the defined Working Range accordingly.

3. New Flag #

Flag # is automatically set for results with CV outside the acceptance limit for double assays in IA projects.

4. Another acceptance criterion

Intercept acceptance criterion added

5. Statistics for CALs/QCs

„Not accepted batches“ (Batch Flag N) can be included in the statistics if necessary

6. Incurred Samples

%-difference can be calculated also in % of the FIRST value .

Reassays can be sorted also according their batch number (sort was according the meas. date so far only)

Result number format for Incurred Samples may be different as the number format of the standard reassays

7. QC and QA

QC Check and QA Reviews are tracked in dbLabCal electronically (date, user and all details in audit trail).

Therefore, paper printout is not necessary to document QC/QA.

+ small bug fixes

Update dbLabCal V3 SP4-> dbLabCal V3 SP5

(May 2008)

1. dbLabCal imports data from Magellan, Access2, FACS, ISE and ELAN-ICP

Data import from another 5 instruments possible.

2. Additional acceptance criteria

New criteria are: Count of accepted QCs and acceptance (cv) for double assays (because of Magellan, Access2 methods)

3. Intra-Day Statistics for CALs is possible

Intra-Day statistics for CALs is calculated and printed if more than one CALs were analyzed in a batch and if the user has chosen the option. That was possible for QCS sample only until now

4. Printouts according GLP-Terminology

The terms „Study Director“, „Principal Investigator“, „Study“ and „Project“ are now used according GLP terminology

5. Not used VAL samples are listed in „Not Used Chromatogramms“

Only not used CALs and QCs were listed until now

6. VAL sample evaluations improvements

Solutions Stability, Matrix-Tests and Carry-Over calculations are possible directly in dbLabCal.

7. Electronic Signature

ES for sample name editing is required after batch status was set

8. Archived Projects

Archived projects are again accessible to the user (with ReadOnly) without „lending out“ procedure.

9. HoLaRo-Reassay rule changed according to current HoLaRo SOP

10. Results of Incurred Samples implemented

11. Planning and results of long term stability experiments

+ small bug fixes

Update dbLabCal V3 SP3-> dbLabCal V3 SP4

(November 2006)

1. New rules for choosing final results from reassays samples added

There are two new rules for choosing reassays (in addition to the existing dbLabCal standard and the Lang&Bolton rule)

- report first accepted result
- report result according HoLaRo rule

In addition, it is possible to apply a rule to one analyte only

2. Import of SoftMax Pro data

It is possible to import SoftMax Pro data in the batch import dialog.

3. Stability calculations also with Peak Area and Peak Height possible

Originally, only the calculated concentration or the current readings (p.a.r. or p.h.r.) was used.

It is now possible to choose the peak area or the peak height, too.

4. S-Flag overwrites the <, > and + flag

Originally, internal standard acceptance check was performed on Y-flagged chromatograms only. From now on, also those chromatograms will get the S flag, which would originally be flagged with <, > or + . The reason is that, in most cases, a internal standard problem would be the cause for setting the <, > or + flag. It means, the priority of the S flag changed. S Flag has higher priority than <, > and + flag.

5. V-Flag samples are listed in „Samples To Be Re-Analysed“

V flag was originally used to document that there is no valid result since there was not sufficient sample volumen do perform the (re-)assay. Now, V flagged samples are listed in „Samples To Be Re-Analysed“ since it may happen that next aliquot can be sent by sponsor and thus the sample can be (re-)assayed

6. Audit Trail View

Audit trail view is reduced after double click in Audit Trail view on some entry in the Action column just to the chosen action type entries. It improves the readability. Standard Audit trail view is restored after repeated double click on the column.

7. Batch List View Filter

A filter is available after CTRL + double click in the column NAME which allows to show and hide the sample types (CAL, QCS, VAL, SUB, SSS and DIV) in the batch list view.

8. Archived Studies

Archived study can be loaded only if the archivist (readonly user with “archive” authorization) has lent it out

9. External ReadOnly User

Externer ReadOnly User was created with ReadOnly access ONLY to studies which were assigned to the external user explicitly.

+ small bug fixes

What's new in dbLabCal V3?

Update dbLabCal 2.1 SP5 -> dbLabCal V3 SP3

(December 2005)

ES

1. The biggest change is that dbLabCal V3 fulfills CFR21Part11 requirements.

That means:

- User has always to login
- dbLabCal locks user automatically if there is no activity during certain period of time (default 30 min.)
- Password has to be changed periodically (default 60 days)
- Password has to fulfill security requirements (not trivial, combination of characters and numbers)
- Electronic signature (ES = user ID+password+reason for change) is necessary after following Actions

Action	ES	Comment
project created		
project edited	X	
access granted to user	X	
regression model changed		
regr.model readings changed		
regr.model weighting changed		
acceptance criterion changed	X	
project status to STARTED		
project status to FINISHED		
project status to RELEASED		
project data exported to *.bio		
project status re-set	X	
batch data imported		
batch number/unit changed	X	
batch start date changed	X	
chrn. flag changed		
chrn. name changed	X	
batch re-calculated		
batch status changed	X	ES only if seq. excluded
final result chosen		
review started		
review finished		

2. System name and batch number changes are possible only in „Date of Analyses“ view due to required ES entry.

Settings

3. It is possible to copy ALL SETTINGS (all data in sub-menu Setting) from existing project into current project in the Project-New... and Project -Edit... dialogs.
4. Acceptance criteria extended. Further, „IS check“ option was included into Acceptance criteria dialog. dbLabCal sets flag S automatically for all SUB samples, if their IS area (or height) is outside the set acceptance criterion.
5. Import and Export path (directories) can be set in a new dialog. (In V2.1 was only one path, which was set automatically after each successful import to the current import path.
6. SUB samples naming type (SUBJECT / PERIOD / TIME or SUBJECT) can be set for project by the user. (In V2.1 dbLabCal set it automatically based in found SUB samples names)

Results

7. Additional QC statistics, including also E-flagged QC samples, is calculated and shown if one or more QC have flag E.
8. It is possible to calculate and show QC statistics „ALWAYS INTRA DAY“. It means intra day MEAN, SD and CV is calculated for all batches and not only for one batch with the highest QC count.
9. There are now 20 groups for Stability/Validation samples (V2.1 had 9 groups).
10. More precise choice for 0-values for Stability/Validation samples is possible.
11. Final results are set through a dialog in „Reassayed Samples“ view.
12. While setting the final results , the current user grants are considered. It means for example than an „Analyst“ cannot overwrite a „Study Directors“ choice. User name of the user who set the final result is displayed in tool tip.

Data Import

13. There is just one import dialog for all import file types - and an additional dialog for direct import from Millennium.
14. It is possible to import any peak count (max. 10 peaks/chromatogram) only at the first import. After that, dbLabCal allows the import only for correct peak count (and peak assignment)
15. It is possible to exclude individual chromatograms from the import in the Import check dialog.

Others

16. Deviation from the nominal concentration [dev %] is shown in the batch list view for all CAL-, QCS- and VAL samples.
17. It is possible to select individual subjects for printing. In V2.1 it was possible only to print all subjects data.
18. It is possible to show and use up to 9 re-assays. In V2.1 it was limited to max. 3 re-assays.
19. Random Repeats: New dialog for „Random Repeats“ added. It is possible to select „Random Repeats“ (click on Option-Button in Results-Subject Samples) directly in dbLabCal. „Random Repeats“ samples have to be are marked in the Batch List view (select chromatograms, press CTRL-R). All „Random Repeats“ samples and results with „Random Repeats“ samples involved are shown (in Results, Subject Samples , Results, Re-Assayed Samples and in batch list) with yellow background.
20. Chromatogram Flag I: New chromatogram flag (I, as Ignore) was created. Now, it is possible to distinguish between „not existing sample“ („missing“) and „received, but not analyzed sample“ by assigning the I flag to a „dummy“ SUB sample. It is then reported in Results, Subject Samples as „Sample received but not analyzed“ (=NOA) instead of „missing“ (=NOS).
21. It is possible to edit chromatogram flags for ALL SELECTED (and visible) chromatogram/analyt rows. It saves few clicks, if for example all results of only one analyte should be set to X flag.
22. dbLabCal shows automatically (only!) the changes (Audit Trail) performed on the current project by another user since current users last logout.