Release Notes

QuBAS Version 2.0.2 build #99

Changes from Version 2.0.1 release

Upgrade advice:

QuBAS version 2.0.2 is a minor upgrade release.

2.0.2 contains many small changes to the user interface designed to make it more intuitive, especially for first time users. These include "hover over" type on screen help boxes and re-labeling of options. (The original names for these re-labelled options are retained in the hover over help for compatibility with client SOPs that may mention the original names).

Some other changes have been made to the underlying infrastructure and admin functions to improve performance with large import files and large numbers of methods and or reports.

There are no changes to the Relative Potency analysis engine. The Interpolation analysis engine has had minor changes to improve Diverse Self-Checking Pair matching for samples with values close to the asymptotes, A change in reporting threshold for un-reliable results and improved error messages.

Quantics advise that on-site upgrade validation is not required but *can be run if desired from the audit login.*

1. End User upgrade validation process

1.1. The validation report shows more details.

To provide extra confidence in the backward compatibility, the report produced by the upgrade validation process now includes the number of individual values compared as well as a pass / fail statement.

E.g: Example of a check of 10 analyses: 11,314 values were compared, and all were identical.

1 Results

Method	Run Name	File Name	Original Run Date	Original Version	Number of Values Compared	Result
Q001 Demo 4pl	tyytjty		10/09/2019	2.0.1	1913	PASS
C1427 Optimisation 2	AutoImport-29/Oct/19 10:58		29/10/2019	2.1.0	1843	PASS
QuBAS tutorial RP analysis	Demo Routine run		02/12/2019	2.0.2	1918	PASS
C1406 AAV	TD 10 and 11 exact doses		09/09/2019	2.0.1	798	PASS
C1406 AAV	TD 10 and 11 exact doses		09/09/2019	2.0.1	799	PASS
CT003 for demo	test run		12/09/2019	2.0.1	1934	PASS
C1634 Validation study October 2019	10 Oct files 50,50,100,100		11/10/2019	2.0.1	527	PASS
C1634 Validation study October 2019	10 Oct files 50,50,100,100		11/10/2019	2.0.1	527	PASS
C1634 Validation study October 2019	10 Oct files 50,50,100,100		11/10/2019	2.0.1	527	PASS
C1634 Validation study October 2019	Plate 2 for 10 Oct run 50%		11/10/2019	2.0.1	528	PASS
		moved_1.csv		Total:	11314	PASS

2 Overall Result

PASS: all the analyses listed produced the same results in version 2.0.2 when compared with the original analyses. Backward compatibility confirmed.

1.2. Interpolation analyses now included in User upgrade Validation process

Audit users can now select a mixture of RP and IA analyses to run with the validation check process.

Change in threshold for acceptance of valid result.

1.3. Change in result precision threshold

The IA engine calculates the confidence intervals of all results, and reports the fold precision, upper CI/ lower CI. To prevent the reporting of results that should not be relied upon, the threshold for reporting was originally set to FP= 10^4. Following discussion, this has now been reduced to 10^3. As a result of this change there are some cases where the FP is between 10^4 and 10^3 that 2.01 reports a value (with the CI) but 2.02 reports "un-reliable". A validation run will produce some mismatches if an FP happens to fall between 1000

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and 10 000. In these cases, a result with such uncertainty would (should) have failed the sample so the impact is negligible.

2. User interface improvements

Many small changes have not been listed individually in these Release Notes but will be obvious to established users. First time users should find the system easier to navigate and use.
Key points include:

- Hover over tool tips in many areas.
- File Importing:
  - The import file template creation screen can now handle take large CSVs. It has been tested with CSV files up to 300 rows and 40 columns (12,000 cells).
  - QuBAS import systems now automatically pads empty rows. E.G: If a Template is expecting 12 rows but the data set only contains 10 (perhaps because of missing data) the system will add 2 blank rows so that the template will work correctly.
  - Template creation now shows alphabetical and numeric numbering for rows and figures.
  - The state of all the auto-import folders can now be seen on one page by Admin users. Log in, select System- Auto import:
    Each folder is classified as:

    Key:

    ✅ The folder is enabled, reachable and there are tokens available.
    ❌ The folder is enabled but not reachable.
    ⚪ Any other situation.

- Data Map (plate map)
  - Plate map substances now ordered by type to aid selection.
  - Plate map substance colors now internally consistent.
- The User list in the Admin section now shows any locked-out users and the super user email address for reference.

- The monitoring room is now available to Routine Users directly from the Routine Room Results page.

- Analysis definition page
  - Options in Analysis page now have increased separation to aid selection.
  - Default values for Goodness of fit F test and parallelism F tests changed to 0.01.

3. Performance

- A pagination process has been added to the following rooms to improve performance when there are large numbers of data files:
  - Import Room
  - Audit Room
  - Monitoring Room

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- Routine Results Room
- Backup database size of 5GB limit now removed
- Hash checks for data integrity now performed at database level rather than at web site level (much faster).

4. System outputs

Results now available as pdf, formatted excel, and xml for LIMS system upload.

5. Additional GMP / CFR 21 part 11 functions

- When dual sign off is selected, the two signatures must be from different users.
- Second signer must enter their PIN for every signature (CFR 21 requirement)

6. Bug fixes

The following bugs have been fixed:
- Occasional unpredictable behavior when deleting elements of the Data map.
- Sending a second version MCF for 2 stage sign off and completing the first sign off locked Users from the Method in Routine Mode. Access now normal.
- Some numbers in the excel output were formatted as text. Now correctly formatted as numbers.
- Development record held wrong User ID in certain circumstances. Now corrected
  - All other ID records were correct, the Report IDs were correct.
- In some circumstances the first file imported into a new Method did not appear on screen until after a refresh. Now fixed.
- In the development record, the results only showed in half the screen. Now fixed.
- Method deletion error now fixed.
- Excel report skipped the wrong number of columns if there was a singular fit resulting in in some sample names in the wrong column.
- In Explore mode, a Save of the analysis definition failed to save the working copy.
- Interpolation Analysis: Reference concentrations can now include zero.
- Previous versions allowed Logging in to a mode that was not authorized for that User. No actions were possible, but the situation was confusing and used a licence. Access now restricted at Mode level rather than actions level.

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7. Update backward compatibility testing

Relative potency

The relative potency analysis engine has not been changed in any way. Backward compatibility was tested with 500 analyses for each of the 5 models (linear, 4pl, 5pl, probit and logit). The results were identical – checked by MD5 #checksums.

Interpolation analysis:

DSCP testing:

16,000 tests run. 381 created a DSCP mismatch (2.3%) all with the 5pl fit. Of these, 370 were deliberate singular fits or random input datasets, designed to fail in most situations.

Overalls realistic mismatch rate = 0.07%

Testing 2.01 Vs 2.02.

Approximately 7000 data sets were tested including extreme random data expected to fail analysis, each set containing a different number of data samples.

QuBAS 2.0.2 is much more robust for datasets with responses near the asymptote (4PL) and this creates more passes in 2.02.

model	2.0.1 and 2.0.2 are equal	Fail in 2.0.1, Run in 2.0.2	Run in 2.0.1, Fail in 2.0.2	Fail in 2.0.1, Fail in 2.0.2	Both Run, results equal but reported differently	total
FivePL	1793	9	0	357	181	2340
FourPL	2129	298	1	7	313	2748
Linear	1998	0	0	0	2	2000
Sum	5920	307	1	364	496	7088
% of total	84%	4%	0.01%	5%	7%	0%

For *backward* compatibility the conservative test is that the numerical results were equal (6780/7088), or the test ran in the new version but did not run in the old (307/7088). 7087/7088 = 99.98% of tests passed this rule. One test initially failed in 2.0.2 but passed in 2.0.1. This was investigated and found to be due to technical issue (not connected with QuBAS directly). When re-run, this dataset ran in both 2.0.1 and 2.0.2.

7% of tests had numerically equal results but *reported* differently due to the change in reporting threshold as noted above. All these had fold precision (upper CI/lower CI between 1000 and 10,000 and would in practise have been un-usable results. However, should this be an issue please contact Quantics who can obtain the actual numbers for these un-reliable results if required.

Backward compatibility testing passed.

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8. Known Issues

1) Some special characters get changed in the UTF8 character set. For example, the character 'α' turns into an 'a' when used in:
- imported files name,
- metadata name,
- template name, or
- metadata content set through the UI.

Workaround: Avoid special characters in metadata if possible. If used, check that they have been imported correctly. Fix issue 2.1.0

2) Some pdf readers will display a message about a missing font. The report display defaults to another font in some areas with no consequences on results or readability. Fix issue 2.1.0

3) Minor GUI issues.

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