



Release Note Summary

QuBAS 3.1.0

07 September 2023

FileHold ID: 1785

FH Version: 2

Approved: See metadata

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Version / Release	07 September 2023
3.1.0 Introduction	3.1.0 is a minor release containing some useful new functions and some bug fixes.
3.1.0 Upgrade advice and versions supported	<p>3.1.0 is a recommended but not required upgrade from 3.0.1. It contains new functions and a number of bug fixes (none of which impacted the reported results). There are changes to some of the analysis components so re-validation is recommended. This can easily be done using the in built revalidation tool.</p> <p>From this release, the supported versions of QuBAS are:</p> <ul style="list-style-type: none"> ❑ 3.0.0 ❑ 3.0.1 <p>If you require help or advice about upgrade please contact support@quantics.co.uk</p>
3.1.0 New features	<p>Analysis options</p> <ul style="list-style-type: none"> ❑ Pseudo replicate handling: Users can now choose to have replicates treated as pseudo replicates if required. When selected, the responses for the replicates are averaged <i>before</i> analysis to ensure the correct calculation of confidence limits. See https://www.quantics.co.uk/blog/understanding-true-replicates-and-pseudo-replicates-in-bioassay/ for further explanation. ❑ R² (coefficient of determination) is now available for 4pl and 5pl models as a goodness of fit measure. <u>Important note:</u> R² has been included following requests from a number of users to allow legacy methods from other systems to run in QuBAS. Statistically, R² is not a valid measure of goodness of fit for linear, 4pl or 5pl models , and its use is not recommended. See https://www.quantics.co.uk/blog/r-we-squared-yet-why-r-squared-is-a-poor-metric-for-goodness-of-fit/ for further details.

	<p>Data file handling</p> <ul style="list-style-type: none"> ❑ A zip of the original file is now stored in the database together with the output of an import plug. Previously, only the output of the plug was stored. ❑ Previously, if a Routine analysis used a plugin, the information about the original file (filename, MD5) was not shown when the analysis is run as a manual run. From this release, if a method uses a plugin, the MD5 and the name of the original file is always shown. <p>Audit functions</p> <ul style="list-style-type: none"> ❑ An Audit User's sign off comments now appear in the full report, not just the interface. ❑ An Audit User can now reject a report with comments. Previously, the only way for an auditor to reject a report was just to not sign it. ❑ If there are no sample in a data file, a report is still produced for audit purposes. <p>User interface</p> <ul style="list-style-type: none"> ❑ Setting up a new sample can be done without switching context (sample mode and metadata mode)
3.1.0 Bug fixes	<ul style="list-style-type: none"> ❑ Pre-dilution factors were not operational in 3.0.0 or 3.0.1 ❑ QuBAS regularly scans all the active auto import folders for Routine Methods. Previously, if a folder in the list was not accessible or did not exist, the process exited and the rest of the folders were not processed and the files in them were never picked up. This has been fixed. ❑ The communication between the user interface and analysis engine failed in certain situations where there were samples that contained no data. This has been fixed. ❑ On screen data plots in the developer mode were set to 0 (zero) for missing data. This was an on screen error only, and the analysis report was not impacted. Fixed ❑ Auditor comments truncated in pdf reports. Fixed ❑ DSCP mismatch when using 5pl models with studentised outlier detection. Fixed

	<ul style="list-style-type: none"> ❑ CSV parser had different levels of format requirements in developer and Routine mode. Leading to some data files running in Developer, but not Routine. Fixed ❑ Other minor bug fixes, none of which impact the analysis results.
3.1.0 Known Issues	<ul style="list-style-type: none"> ❑ The logging out message from the development room only disappears with a screen refresh ❑ QuBAS fails to load data files with a path name >260 characters due to Windows default settings. Keep filenames and path to < 260 characters.
3.1.0 Testing	<p>The analysis engines have been updated and therefore a full testing program has been undertaken at Quantics.</p> <p>Technical DSCP tests:</p> <ul style="list-style-type: none"> ❑ Approximately 72,000 datasets have been used (291 classes of datasets, each generating about 250 datasets). Some datasets are specifically designed to stress the engine and are not expected to yield 100% DSCP match. The results are compatible with previous releases. <p>User testing:</p> <ul style="list-style-type: none"> ❑ 78 User stories (test cases that are user testable) have been checked twice, by 2 different non-technical Users. <p>Backward-compatibility testing</p> <ul style="list-style-type: none"> ❑ About 500 test cases for all models were run with the Analysis engine of QuBAS 3.0.1 and QuBAS 3.1.0 and the results were compared. The test cases were realistic datasets with random perturbations (e.g. outliers etc.) and involve >500,000 DSCP tests.

	<div><div><div>RP analyses</div><table><thead><tr><th>Model</th><th>Works in 3.0.1</th><th>Works in 3.1.0</th><th>Results are equal</th><th>n (%)</th></tr></thead><tbody><tr><td>Five PL</td><td>FALSE</td><td>FALSE</td><td>NA</td><td>3 (0.61%)</td></tr><tr><td>Five PL</td><td>TRUE</td><td>TRUE</td><td>TRUE</td><td>488 (99.39%)</td></tr><tr><td>Four PL</td><td>TRUE</td><td>TRUE</td><td>TRUE</td><td>500 (100.00%)</td></tr><tr><td>Linear</td><td>TRUE</td><td>TRUE</td><td>TRUE</td><td>500 (100.00%)</td></tr><tr><td>Logit</td><td>TRUE</td><td>TRUE</td><td>TRUE</td><td>496 (100.00%)</td></tr><tr><td>Probit</td><td>TRUE</td><td>TRUE</td><td>TRUE</td><td>496 (100.00%)</td></tr></tbody></table></div><div><div>IA analyses</div><div>IA analyses</div><table><thead><tr><th>Model</th><th>Works in 3.0.1</th><th>Works in 3.1.0</th><th>Results are equal</th><th>n (%)</th></tr></thead><tbody><tr><td><u>FivePL</u></td><td>TRUE</td><td>TRUE</td><td>TRUE</td><td>495 (100.00%)</td></tr><tr><td><u>FourPL</u></td><td>TRUE</td><td>TRUE</td><td>TRUE</td><td>500 (100.00%)</td></tr><tr><td>Linear</td><td>TRUE</td><td>TRUE</td><td>TRUE</td><td>500 (100.00%)</td></tr></tbody></table><div><div></div><div>The results are equal across version. There are 3 datasets for which the analysis failed, in both version. Those are extreme datasets which are mathematically unstable with a 5PL fit.</div></div></div></div>	Model	Works in 3.0.1	Works in 3.1.0	Results are equal	n (%)	Five PL	FALSE	FALSE	NA	3 (0.61%)	Five PL	TRUE	TRUE	TRUE	488 (99.39%)	Four PL	TRUE	TRUE	TRUE	500 (100.00%)	Linear	TRUE	TRUE	TRUE	500 (100.00%)	Logit	TRUE	TRUE	TRUE	496 (100.00%)	Probit	TRUE	TRUE	TRUE	496 (100.00%)	Model	Works in 3.0.1	Works in 3.1.0	Results are equal	n (%)	<u>FivePL</u>	TRUE	TRUE	TRUE	495 (100.00%)	<u>FourPL</u>	TRUE	TRUE	TRUE	500 (100.00%)	Linear	TRUE	TRUE	TRUE	500 (100.00%)
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3.1.0 Build	<div><div></div><div>3.1.0_66.</div></div>																																																							
3.1.0 Installer Checksums	<div>The installer is QuBAS_3.1.0_66.exe</div> <div>The MD5 is: 8CE0E052F20EF5FA47C95BAA19BD692D</div>																																																							