



Release Note Summary

QuBAS 3.0.1

06 September 2022

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Version / Release	29 July 2022
3.0.0 Introduction	<p>QuBAS 3.0.0 is a major upgrade, primarily in response to user feedback. Users had requested more flexibility for use in early stages of assay development, and a more intuitive interface. In addition to the interface changes we took the opportunity to undertake a major upgrade of the QuBAS infrastructure.</p> <p>The result is a much more flexible Explore room – now called Developer- and significant improvements to speed and robustness to external network interruptions.</p>
3.0.0 Upgrade advice	<p>3.0.0 is a recommended upgrade. It will be possible to upgrade from 2.0.x directly to 3.0.0.</p> <ul style="list-style-type: none"> ❑ QuBAS 3.0.0 only supports MSSQL. If you use MySQL or Local DB from previous versions contact us for upgrade support. <p>Some changes in 3.0.0 are not backward compatible. See Upgrade information for further details.</p> <ul style="list-style-type: none"> ❑ From the Launch of 3.0.0, free technical support is only available for 3.0.0, and 2.1.1 <p>How to upgrade:</p> <ol style="list-style-type: none"> 1) Login as system administrator and create a database backup from within QuBAS. <ol style="list-style-type: none"> a. We recommend you also take a direct database backup. 2) Download and Run the 3.0.0 installer. This will: <ol style="list-style-type: none"> a. Download all the required files for 3.0.0 b. Migrate the original 2.x.y database to the new 3.0.0 structure.

	<p>c. Install all the files and the new migrated database.</p> <p>3) Login as audit user to Audit room</p> <p>4) Lock off Routine mode</p> <p>5) ...run validation process</p>
3.0.0 New features	<p>Developer Mode (previously “Explore”)</p> <p>User Interface</p> <p>3.0.0 has a completely new user interface. A few of the key features are noted here.</p> <ul style="list-style-type: none"> ❑ The previous work flow of: <p>Load data file, create Data File Template, create Data map, add dilutions, ...has been replaced by a single screen. The required information can be added in any order, simply by drawing onto the data file.</p> ❑ No need to specify Substance and Method metadata when creating a Method ❑ Analysis can be run without metadata – leave this until later in development if you wish. ❑ Some other features: ❑ Draw in a sample, hover over to show dose or response:

Manual metadata: None ([Create](#))

#	1 (A)	2 (B)	3 (C)	4 (D)	5 (E)	6 (F)	7 (G)	8 (H)	9 (I)
1 (A)	ref	REF							
2 (B)	test1	TEST1							
3 (C)	test2	TEST2							
4 (D)	date	25/11/...							
5 (E)									
6 (F)									
7 (G)									
8 (H)									
9 (I)									
10 (J)									
11 (K)	conc	1	2	3	4	5	6	7	8
12 (L)									
13 (M)		7.8	7.3	6.1	5.1	3.3	2.2	2.1	2.2
14 (N)		7.6	7.4	6.5	4.7	3.8	3	2.4	2.1
15 (O)		7.7	7.1	6	4.6	3.3	2.5	2.4	2.2
16 (P)		7.5	7.3	6.5	4.9	3.2	2.4	2.1	2.2
17 (Q)		7.2	6.2	4.9	3.5	2.4	2.1	2	1.9
18 (R)		7.1	6.5	4.3	3	2.7	2.3	2.1	1.8

#	1 (A)	2 (B)	3 (C)	4 (D)	5 (E)	6 (F)	7 (G)	8 (H)	9 (I)
(A)	ref	REF							
(B)	test1	TEST1							
(C)	test2	TEST2							
(D)	date	25/11/...							
(E)									
(F)									
(G)									
(H)									
(I)									
0 (J)									
1 (K)	conc	1			4	5	6	7	8
2 (L)									
3 (M)		1	2	3	4	5	6	7	8
4 (N)		1	2	3	4	5	6	7	8
5 (O)		7.7	7.1	6	4.6	3.3	2.5	2.4	2.2
6 (P)		7.5	7.3	6.5	4.9	3.2	2.4	2.1	2.2
7 (Q)		7.2	6.2	4.9	3.5	2.4	2.1	2	1.9
8 (R)		7.1	6.5	4.3	3	2.7	2.3	2.1	1.8

- Copy and paste samples, doses, whole plate maps
- View mode reorganises any data layout into easy-to-read standard format:

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Design your Data Map

EditView

Name	Type	Value	Name	Type	Value	Name	Type	Value
Operator ID	Text	CL	Reagent ID	Text	R003	Test date (m...	Date - DMY	-
Name	Type	Identifier						
ref	Reference	Ref 001	-	dose: 0.04882...				
				0.01932...	0.00271...	0.03675...	0.02119...	0.14055...
Sample 1	Test Sample	TS 1	-	dose: 0.04882...				
				0.03905...	0.03278...	0.03353...	0.04221...	0.33215...
Sample 2	Test Sample	TS2	-	dose: 0				
				Ref 001				

☐ Read pre-dilution factors dynamically from the data file:

- Add a Metadata marker, and select Type Pre-Dilution, and the sample it refers to:

TY 4pl take 2

Quantitative

Save version

Design your Data Map

Edit View

Datafile: dataset_2 1é_1.csv (change)

Separator: Comma (',') (change)

Unit: (change)

Manual metadata: None

1.5

What is it? Predilution

Which sample? Sample 2

#	1 (A)	2 (B)	3 (C)	4 (D)	5 (E)	6 (F)
2 (B)	Assay date	10/12/20...				
3 (C)						
4 (D)	Operator...	CLÉaíúé				
5 (E)	ReagentID:	R003				
6 (F)						
7 (G)	Sample i...					
8 (H)						
9 (I)	Sample n...	Sample t...		Predilution		
10 (J)	Ref	0		1		
11 (K)	Test01	TS 1		Sample 2 Test Sample		
12 (L)	Test02	TS2		1.5		
13 (M)	QC01	Q-xyz				

- Manage Metadata view organises the metadata:

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Manage your Metadata

Datafile: dataset_2 16_1.csv

Sample Metadata

Name	Type	Identifier	Predilution
ref	Reference	Ref 001	
Sample 1	Test Sample	TS 1	
Sample 2	Test Sample	TS2	1.5

Other Metadata

Name	Type	Required	File Value	Manual
Test date (...)	Date - DMY	×	-	
Reagent ID	Text	×	R003	
Operator ID	Text	×	CLÉALUÉ	

Quick Fit Analysis

Quick fit analysis will fit the specified model to the data to allow a visual inspection of fit. No need to specify sample type or metadata, just doses and responses. QuBAS provides default label:

01	0-xvz										
Sample 1 Test Sample Dose/Dilution: 25 Value: 2.252179901											
126621...	25	12.5	6.25	3.125	1.5625	0.78125	0.390625	0.1953125	0.097656...	0.048828...	-
103397...	25	12.5	6.25	3.125	1.5625	0.78125	0.390625	0.1953125	0.097656...	0.048828...	(
112750...	4.996749...	5.472208...	4.780386...	3.6821854	1.740106...	0.215597...	0.042395...	0.029870...	0.025247...	0.026385...	(

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Quick fit Full Analysis

2 Explore the results

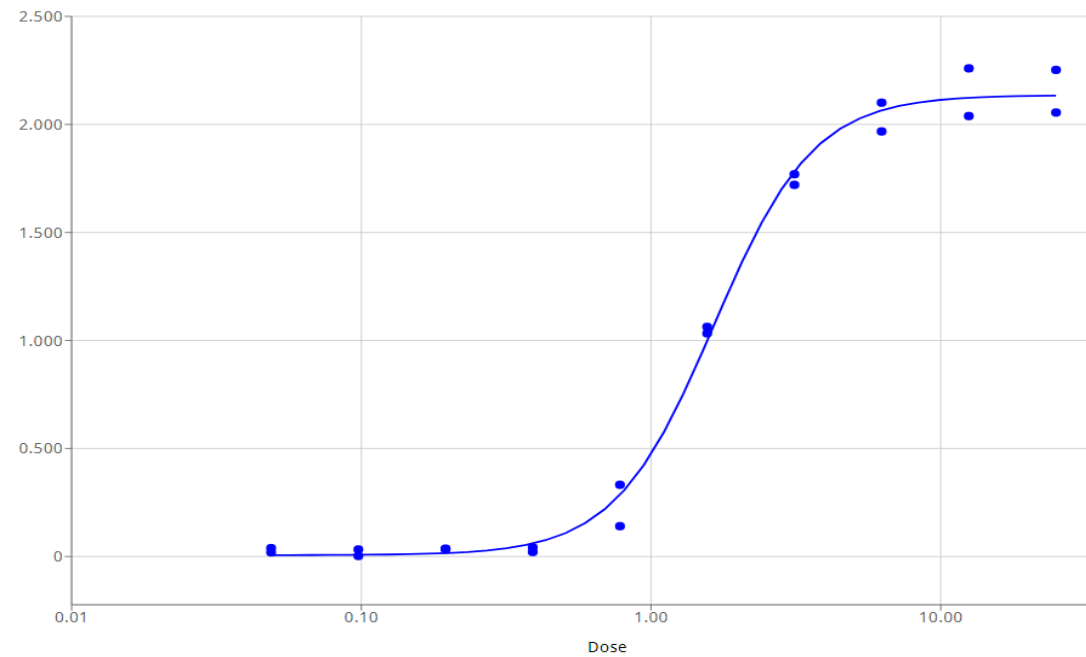
Select Plot Type

Data Plot

Quick Fit

Unconstrained Analysis

Parallel Analysis



Sample 1

On screen graph displays multiple samples, each of which can be shown or hidden:

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QUBAS
BIOASSAY SOFTWARE by Quantics



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QUBAS
BIOASSAY SOFTWARE by Quantics

Development Report

- ❑ The Development report has been replaced by a new version system. In QuBAS 3.0, a 'SAVE VERSION' saves the entire status at that time, including all information in the design page and analysis page, and the data set in use, and reports if available. It is like a system snapshot. The development progress can be shown graphically:
- ❑ Graphical Version history shows predecessor designs:

TY 4pl take 2 Quantitative

Method Version History

Date	History	Default version	Cha
JULY 2022			
24 July 2022 at 11:21:35		<input checked="" type="radio"/> Current	ian.;
24 July 2022 at 10:47:24	●	<input type="radio"/> Open this version	ian.
20 July 2022 at 14:09:03	○	<input type="radio"/>	ian.;
20 July 2022 at 13:38:21	○	<input type="radio"/>	ian.;
20 July 2022 at 10:24:14	○	<input type="radio"/>	ian.;
20 July 2022 at 07:55:25	○	<input type="radio"/>	ian.;
20 July 2022 at 07:46:33	○	<input type="radio"/>	ian.;
20 July 2022 at 07:42:17	○	<input type="radio"/>	ian.;

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Method Version History

Date	History	Default version	Ch
JULY 2022			
24 July 2022 at 11:21:35		 Current	iar
24 July 2022 at 10:47:24			iar
20 July 2022 at 14:09:03			iar
20 July 2022 at 13:38:21			iar
20 July 2022 at 10:24:14			iar
20 July 2022 at 07:55:25			iar
20 July 2022 at 07:46:33			iar
20 July 2022 at 07:42:17			iar

- When saving notes are available to record changes. Use Auto notes to provide headings for detail.
- Notes are shown in version screen
- The development report in PDF is clearer and contains a snapshot of the plate map, metadata and plots.

Monitoring Room (Trending)

- Trending is now only available with a Routine license
- Improved filtering
- When accessed with a Routine license, saved Developer analyses can be displayed and the associated report downloaded direct from the trending plot.

Report changes

- ❑ In earlier versions, the imported file “Date of last modification” date picked up from Windows file systems was reported in the Routine report audit trail. However, this date can be misleading as it may even be before date of creation. To avoid this confusion, the data has been removed.
- ❑ If it is not possible to fit the data a report is still produced with data plot and an explanation. This is for GMP record keeping purposes.
- ❑ If an analysis fails for a technical reason, such as might occur if the two branches of the Continuous real-time Validation do not match, an informative pdf report is still produced for GMP audit purposes.

Routine Room

- ❑ Combined RP tab now shows which samples were included in historic runs:

Method: test-4pl + Create Combined Report					
Report ID		MCF Version		Run By	
9		1		sandra.quickert@quantics.co.uk	
Run Name	Report ID	Sample	Relative Potency	Lower Bound CI (95%)	Up
AutoImport-25/Nov/19 14:01	7	TEST2	14.10	9.33	
AutoImport-25/Nov/19 14:01	8	TEST2	23.80	15.63	
-	Combined	-	18.22	13.66	

- ❑ Data Transfer folder log (DTF): When using auto import, errors with files or Plugin errors are now recorded in a log.txt file in the DTF /errored field, and the same information is available in Routine room :

AutoImport-29/Jul/22 06:22

Error log (5)

[29/Jul/22 06:22] Auto Import could not run plugin on file crashA.csv. File moved to \\quantics-server\software development\auto\DSCPTest\errored\crashA_2022_07_29_05_22_06.csv. Branch A has exited with no results.

[29/Jul/22 06:22] Auto Import could not run plugin on file crashB.csv. File moved to \\quantics-server\software development\auto\DSCPTest\errored\crashB_2022_07_29_05_22_06.csv. Branch B has exited with no results.

[29/Jul/22 06:22] Auto Import could not run plugin on file failDSCP_Plugin.csv. File moved to \\quantics-server\software development\auto\DSCPTest\errored\failDSCP_Plugin_2022_07_29_05_22_07.csv. Output of plugin files do not ma

[29/Jul/22 06:22] Auto Import could not run plugin on file notATextFile.png. File moved to \\quantics-server\software development\auto\DSCPTest\errored\notATextFile_2022_07_29_05_22_07.png. Branch A output file is not UTF-8.

[29/Jul/22 06:22] Auto Import could not add file templateIssue.csv to the run, created a copy in \\quantics-server\software development\auto\DSCPTest\errored\templateIssue_2022_07_29_05_21_19.csv.

Name	Report ID	MCF Version	Status	All SSC Passed	Run By
works.csv	20122	1	Complete	Yes	autoimport@autoimport.autoimport

Database validation

QuBAS ensures the integrity of the database by hashing its content and regularly checking its current value against the expected one. This has been redesigned and is now much more robust and less prone to false mismatch errors.

3.0.0 Bug fixes

Improved special character management on screen and in reports

Validation was not possible if the original user had changed email address.

Results were occasionally duplicated in the result accordion on the user interface (routine analysis).

Password expiry used to affect Active Directory users.

The option for systematic validation prior to a routine run was always starting at ‘Yes’ (Admin room)

An email was incorrectly sent when a method was successfully deleted.

Files that failed to AutoImport correctly were not always moved to the errored folder, but went through to the Data Import room and then failed. See also new feature : auto import failure log.

Validation runs now possible if email addresses have changed

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3.0.0 Known Issues	<ul style="list-style-type: none"> ❑ The monitoring room repeats the sample names for each analysis. ❑ With very large databases, the log out process may take more than 1 minute. This is due to the database hashing process which will continue until complete in the background . ❑ Workaround: Refresh the page. ❑ When accessing the help files from within QuBAS, a few of the links fail. The full help file is available on the Quantics website.
3.0.0 Upgrade information	<ul style="list-style-type: none"> ❑ QuBAS 3.0.0 only supports MSSQL. If you use MySQL or Local DB from previous versions contact us for upgrade support. ❑ Data file templates and data maps from earlier versions that were not saved to the Development report will not be available after migration ❑ QuBAS expects .csv files (or other delimiter). There are formal international specifications for such files and QuBAS has been updated to conform to these standards. Earlier versions would occasionally accept some types of poorly formatted CSV files, so if these are present in the database, they will not run in QuBAS 3.0. Contact us if you need help with reading in CSV files. ❑ Quantal models: points with a maximum value of 0 are now considered invalid and not included in the analysis. ❑ SPL models: the fitting procedure for SPL has been improved for situations where the responses are large. The improvement can on occasion impact on fits that are very nearly singular (and thus reporting results of little use, with very large confidence intervals). Those borderline fits may now be considered singular and therefore produce a different result (singular fit vs very unstable) during a validation run.
3.0.0 Testing@Quantics	<ul style="list-style-type: none"> ❑ All testing results available for review – contact us <p>290,000 datasets tested for DSCP functions. Because the curve fitting processes need to use numerical analysis techniques, creating 2 DSCP arms that agree is very difficult (see Quantics blog) For all reasonable data sets we have achieved this. In some very extreme cases not seen in real use, there may be mismatches occurring. These 290,000 datasets are designed to test the extremes and not all are expected to</p>

be create matching results. We are looking to see that the frequency of DSCP issues is broadly the same between versions, rather than matching extreme values across versions. - **Passed**

- Backward compatibility of analysis engines: 500 extreme datasets of each model (RP: 4PL, 5PL, linear, logit, probit, ID: 4PL, 5PL, linear) have been analysed in 2.1.0 and 3.0.0, and their results compared (4,000 total).

The only differences are in 4PL and 5PL. The fitting procedure for 4PL and 5PL has been improved for situations where the responses are large. The improvement can on occasion impact on fits that are very nearly singular (and thus reporting results of little use, with very large confidence intervals). Those borderline fits may now be considered singular and therefore produce a different result (singular fit vs very unstable) during a validation run. In 10/4000 cases, V3.0.0 does not give a result, where V2.1.0 did give a result, and in 5/4000 V3.0 does give a result where V2.1.0 did not.

Analysis	Model	Results 2.1.0	Results 3.0.0	Equal results	n
Interpolation Analysis	FivePL	No	No	NA	8
		Yes	No	NA	2
		Yes	Yes	true	490
	FourPL	No	No	NA	1
		Yes	Yes	true	499
	Linear	Yes	Yes	true	500
Relative Potency	fivePL	No	No	NA	27

		No	Yes	NA	5
		Yes	No	NA	8
		Yes	Yes	true	460
		No	No	NA	1
		Yes	Yes	true	499
	fourPL	Yes	Yes	true	500
	linearModel	Yes	Yes	true	500
	logitModel	Yes	Yes	true	500
	probitModel	No	No	NA	1
	probitModel	Yes	Yes	true	499
<p>Validation testing using QuBAS internal validation process run 29 July 2022 @ 01.04. Run 400 data sets and compares results from 2.02 with those obtained in 3.0. 413,029 numeric checks made – all agree. Backward testing Pass.</p>					

linear demo	12/Apr/21 16:27					
Quantics IA linear demo	AutoImport- 12/Apr/21 16:27	dataset_linear	12/04/2021	2.0.2	632	PASS
Quantics IA linear demo	AutoImport- 12/Apr/21 16:27	dataset_linear	12/04/2021	2.0.2	632	PASS
Total:					413029	PASS

2 Overall Result

PASS: all the analyses listed produced the same results in version 3.0.0 when compared with the original analyses.
Backward compatibility confirmed.

- ❑ Unit testing, integration / build testing. **All pass.**
- ❑ Final User testing: Two independent non-technical users. Seventy one specific, targeted test scenarios designed to test all aspects of the QuBAS system as a real user. **All pass both testers.**

3.0.0 Installer Checksums

The installer is Build 81

The MD5 is: FCD3095A9C197617D9E323535E53A4D0 QuBAS_3.0.0_81.exe

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3.0.1 Introduction	<p>3.0.1 This is a small but required update for those who upgraded to 3.0.0.</p> <p>3.0.1 This is a recommended upgrade or those on versions prior to 3.0.0 and can be installed directly without installing 3.0.0 first</p> <p>3.0.0 introduced stricter controls on CSV formats to comply with international RFC 4180 standards. However it is now apparent that some laboratory equipment does not produce RFC compliant CSV files so some of the stricter controls introduced in 3.0.0 have had to be relaxed slightly. One of the CSV format standards assumed, but not enforced by 3.0.0, has had to be enforced because of the very slight possibility that data files could be incorrectly read. This is the reason for the Required status for users of 3.0.0.</p>
3.0.1 Upgrade advice	<p>3.0.1 is a required upgrade for clients who installed 3.0.0. It is a recommended upgrade or those on versions prior to 3.0.0 and can be installed directly without installing 3.0.0 first. There are no changes to any of the analysis components of 3.0.0 so re-validation is not required if upgrading from 3.0.0</p> <p>If upgrading from 2.x.y then validation may be required according to local SOPs See 3.0.0 release notes above.</p>
3.0.1 Functional changes	<ul style="list-style-type: none"> ❑ Function change resulting in REQUIRED upgrade status: CSVs should have consistent line endings (RFC4180) (CRLF). The new 3.0.0 user interface assumed this was the case but did not enforce it. However it has been discovered that some laboratory equipment does not conform to this and with certain specific <i>combinations</i> of inconsistent line endings the user interface interpreted the row count in a different way from the analysis engine, resulting in a potential row shift and obviously wrong analysis (samples wrong size/missing). <i>This is a rare but important issue so this requirement has now been enforced</i> and inconsistent line endings will result in an error message and no analysis. A standard QuBAS plugin (free) can be used to automatically correct this type of CSV file error. ❑ CSVs should have a rectangular format, with all rows having the same number of columns. Some common laboratory equipment outputs irregular / non rectangular format files which crashed the new stricter user interface. This requirement has been removed.

	<ul style="list-style-type: none"> ❑ The reports showed an error message when a sample contained only zero doses. The reports don't show an error message anymore, and show a plot for this sample.
3.0.1 Bug fixes	<ul style="list-style-type: none"> ❑ 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. ❑ A change in 3.0.0 made it impossible to use some older plugins. This is fixed.
3.0.1 Known Issues	<ul style="list-style-type: none"> ❑ The monitoring room repeats the sample names for each analysis. ❑ With very large databases, the log out process may take more than 1 minute. This is due to the database hashing process which will continue until complete in the background. ❑ Workaround: Refresh the page. ❑ When accessing the help files from within QuBAS, a few of the links fail. The full help file is available on the Quantics website. ❑ Accents in file names may cause reports to have long and apparently meaningless filenames. The report itself is valid and is not impacted in any way. <ul style="list-style-type: none"> ○ Workaround – either don't use accents in filenames, or rename the report file after saving.
3.0.1 Testing	<ul style="list-style-type: none"> ❑ There is no change to any analysis components. Testing at Quantics comprised 4 level specific testing for the issues noted in this release notes.
3.0.1 Installer Checksums	<p>The installer is QuBAS_3.0.1_14.exe</p> <p>The MD5 is: 9604B0314B361AF2CAD513FBB7C9199A</p>

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