

# QuBAS 3.0 QUICK START TUTORIAL



# CONTENTS

|  |                   |
|--|-------------------|
| <b>Login Page</b>                                  | <b>Page 4-5</b>   |
| <b>The Relative Potency analysis workflow</b>      | <b>Page 6</b>     |
| <b>Creating a new method</b>                       | <b>Page 8-9</b>   |
| <b>Importing a data file</b>                       | <b>Page 10-12</b> |
| <b>“Painting” a Plate Map</b>                      | <b>Page 13-22</b> |
| <b>Setting the Analysis Definition and running</b> | <b>Page 23-26</b> |
| <b>Downloading and viewing the analysis report</b> | <b>Page 27</b>    |
| <b>Method version history</b>                      | <b>Page 28-29</b> |



|  |                   |
|--|-------------------|
| <b>Locking &amp; signing off the method</b>      | <b>Page 32-34</b> |
| <b>Setting an Auto Import folder</b>             | <b>Page 35-37</b> |
| <b>QuBAS routine (Relative Potency) GMP mode</b> | <b>Page 38-43</b> |
| <b>The Monitoring Room</b>                       | <b>Page 44-45</b> |
| <b>QuBAS Interpolation Analysis (IA)</b>         | <b>Page 46-54</b> |



## License

Please select required mode of operation

Development Mode

Routine Mode

Audit and second sign off access

Admin

0/2

Licences in use

## Log in

Please enter your account credentials

Email

Password

[Change Credentials](#)

Log in





- ❑ The 2 data files required for the tutorial can be downloaded here:  
[www.quantics.co.uk/qubas-bioassay-software/quick-start-guide/](http://www.quantics.co.uk/qubas-bioassay-software/quick-start-guide/).
- ❑ Select the licence mode
  - *Development mode* – for setting up and developing an analysis
- ❑ Enter the login details you set up in response to the QuBAS invitation email - your email address, password and PIN number  
NB: the PIN number is an extra security feature that may not be enabled on all systems



## 1) Create Method

- Define a name and what dataset type it is (i.e. quantitative, quantal or interpolation analysis)

## 2) Import data file

- Browse to a .csv data file

## 3) Design your plate map

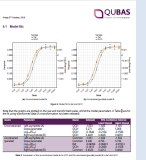
- Design your plate map including doses, sample locations and metadata on top of your dataset

## 4) Select model type and 'Quick Fit'

- Select your model type and run a 'Quick Fit' analysis for instant results

## 4) Select analysis options and run

- Select additional suitability criteria if necessary and once run, a full report is produced.





# The 4 steps (shown above) are required to set up and run a new Relative Potency analysis

These 2 steps:

1) Create Method

2) “Paint” Plate Map

... are only performed once (unless data format changes)



### Method

Please select an existing method to use, or create a new one.

Create New Method +

### Recent

|                            |                        |
|----------------------------|------------------------|
| CT011 <small>(GMP)</small> | Interpolation Analysis |
| CT028 <small>(GMP)</small> | Interpolation Analysis |
| CT040                      | Interpolation Analysis |
| EH IA 5PL                  | Interpolation Analysis |

☒ All
 ☐ Quantitative
 ☐ Quantal
 ☐ Interpolation Analysis

|                            |                        |
|----------------------------|------------------------|
| CT024                      | Quantitative           |
| CT025                      | Interpolation Analysis |
| CT026                      | Interpolation Analysis |
| CT027 <small>(GMP)</small> | Quantitative           |
| CT028 <small>(GMP)</small> | Interpolation Analysis |
| CT029                      | Quantitative           |

Please select a method.

Use this method ↗



# 1) CREATE NEW METHOD

- ❑ Select *Create new Method*
- ❑ Enter an identifiable name for your new method
- ❑ Select *Quantitative* – for Linear, 4PL, or 5PL parallel line analyses
- ❑ Click *Save*.



## Design your Data Map

[Edit](#) [View](#)

Datafile: ( [select data file](#) )

Separator: Comma (',' ) ( [change](#) )

Unit: ( [change](#) )



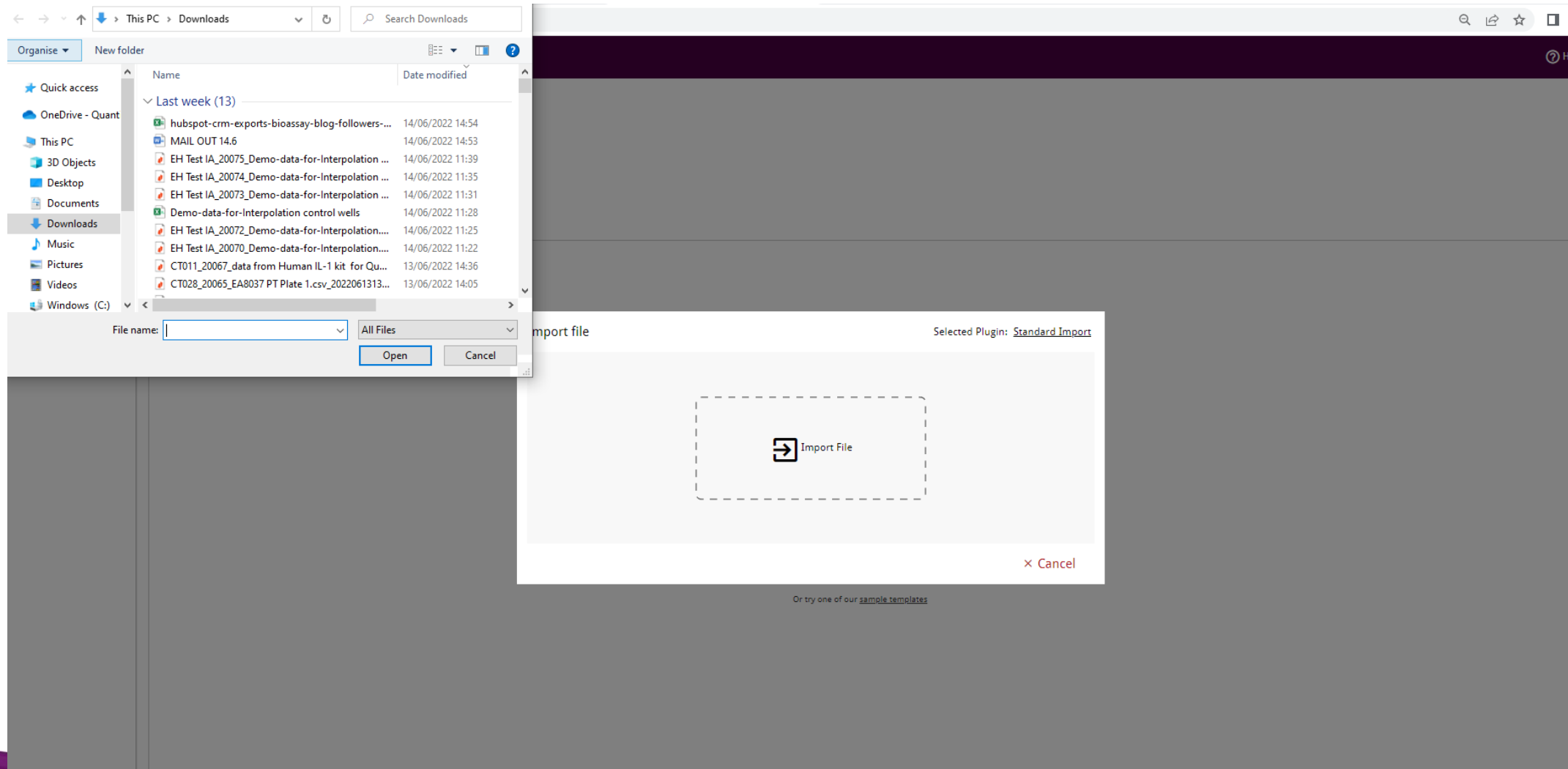
Manual metadata: None ( [Create](#) )

IMPORT A DATA FILE



Or try one of our [sample templates](#)







## 2) IMPORT A DATA FILE

- ❑ Select *Import a Data File* or *Select a Data File* from the middle of the plate map or the top of the page
- ❑ Select *Import File* on the next screen. This is automatically set to a Standard Import - *Simple file upload* plugin.
- ❑ Browse to the file named “*Demo data for tutorial.csv*” (for RP) or “*Demo-data-for-Interpolation.csv*” (for IA).

*You may find these in your Downloads folder from earlier.*



## Design your Data Map

Edit View

Datafile: Demo-data-for-tutorial.csv ( [change](#) )

Separator: Comma (",") ( [change](#) )

Unit: ( [change](#) )



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

| #       | 1 (A)       | 2 (B)       | 3 (C)    | 4 (D)       | 5 (E)    | 6 (F)      | 7 (G)   | 8 (H)   | 9 (I)   | 10 (J)  | 11 (K)  | 12 (L)  | 13 (M)  | 14 (N)  | 15 (O) |
|---------|-------------|-------------|----------|-------------|----------|------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 1 (A)   | ##Blocks... |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 2 (B)   | Plate:      | Plate#1     | 1.3      | PlateFor... | Endpoint | Lumines... | Raw     | FALSE   | 1       |         |         |         |         |         | 1      |
| 3 (C)   |             |             | 1        | 2           | 3        | 4          | 5       | 6       | 7       | 8       | 9       | 10      | 11      | 12      |        |
| 4 (D)   |             |             |          | 0           |          |            |         |         |         |         |         |         |         |         |        |
| 5 (E)   |             |             | 0.00611  | 2.49869     | 2.51361  | 1.84246    | 2.05961 | 1.07906 | 0.18576 | 0.03507 | 0.0213  | 0.02312 | 0.02515 | 0.01103 |        |
| 6 (F)   |             |             | 0.01335  | 3.79014     | 4.68657  | 4.3493     | 4.07266 | 2.30186 | 0.38325 | 0.06629 | 0.02609 | 0.0246  | 0.02494 | 0.00538 |        |
| 7 (G)   |             |             | 0.02667  | 6.13374     | 4.48     | 4.65411    | 4.68857 | 2.40562 | 0.4515  | 0.06298 | 0.02762 | 0.02317 | 0.02425 | 0.02206 |        |
| 8 (H)   |             |             | 0.00032  | 1.76234     | 2.32573  | 2.3058     | 1.79709 | 1.12415 | 0.38487 | 0.06129 | 0.03142 | 0.02788 | 0.02856 | 0.0027  |        |
| 9 (I)   |             |             | 4.00E-05 | 1.96571     | 2.47976  | 2.45668    | 1.6681  | 0.75452 | 0.15193 | 0.03745 | 0.02267 | 0.02873 | 0.02725 | 0.00186 |        |
| 10 (J)  |             |             | 0.006    | 5.23174     | 5.15026  | 3.98534    | 3.55127 | 2.31853 | 0.39086 | 0.05767 | 0.02572 | 0.02385 | 0.0224  | 0.00505 |        |
| 11 (K)  |             |             | 0.0057   | 4.46098     | 5.48986  | 4.53127    | 3.59156 | 2.24422 | 0.34404 | 0.06237 | 0.02686 | 0.0221  | 0.02628 | 0.02537 |        |
| 12 (L)  |             |             | 0.007    | 1.78194     | 2.6407   | 1.83201    | 2.02373 | 1.1996  | 0.34977 | 0.06353 | 0.03068 | 0.02375 | 0.02658 | 0.02928 |        |
| 13 (M)  |             |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 14 (N)  | ~End        |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 15 (O)  | Note:       |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 16 (P)  | Assay date  | 12/09/20... |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 17 (Q)  | Assay ID    | MS00712...  |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 18 (R)  | Ref ID      | R345/1      |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 19 (S)  | Control ID  | Cabc/2      |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 20 (T)  | Test 1 ID   | SM001       |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 21 (U)  | Test 2 ID   | SM002       |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 22 (V)  |             |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 23 (W)  |             |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 24 (X)  | QC ID       | Qual586     |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 25 (Y)  | ~End        |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 26 (Z)  | Note:       |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 27 (AA) | Operator    | Ian         |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 28 (AB) | Reagent ID  | Lot20Jun    |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 29 (AC) |             |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 30 (AD) |             |             |          |             |          |            |         |         |         |         |         |         |         |         |        |
| 31 (AE) | ~End        |             |          |             |          |            |         |         |         |         |         |         |         |         |        |



### 3) DESIGN YOUR DATA MAP

#### Locating your response values

- The location of your samples can be selected using the Pointer tool.
- For this demonstration dataset our layout follows:

\*Columns are letters and Rows are numbers

| Label            | Type      | 1 <sup>st</sup> Replicate | 2 <sup>nd</sup> Replicate |
|------------------|-----------|---------------------------|---------------------------|
| Reference        | Reference | D5-M5                     | D9-M9                     |
| Dose response QC | QC        | D8-M8                     | D12-M12                   |
| Control          | Control   | C5-C12                    | N5-N12                    |
| Test Sample 1    | Test      | D6-M6                     | D10-M10                   |
| Test Sample 2    | Test      | D7-M7                     | D11-M11                   |



### 3) DESIGN THE PLATE MAP








- ❑ Click-and-drag the desired locations for the control wells using the Pointer tool.
- ❑ A pop-up will arise asking:
  - *What is this called?* This is for the sample name (this can also be left empty and will be auto populated).
  - *What is it?* This is for the sample type which will allow a selection from a drop-down menu.

**Design your Data Map** Edit View


Datafile: Demo-data-for-tutorial.csv ( [change](#) )





Separator: Comma (',' ) ( [change](#) )

Unit: ( [change](#) )

What is this called?

What is it? Control Well 

    ✕ ✓









### 3) DESIGN THE PLATE MAP

- As the controls have replicates on the plate, the Resize icon here is needed.

ial.csv ( [change](#) )

What is this called? **Sample 1**

What is it?

|    | 3 (C) | 4 (D)       | 5 (E)    | 6 (F)      | 7 (G)   | 8 (H)   | 9 (I)   | 10 (J)  | 11 (K)  | 12 (L)  | 13 (M)  | 14 (N) | 15 (O) |
|----|-------|-------------|----------|------------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| #1 | 1.3   | PlateFor... | Endpoint | Lumines... | Raw     | FALSE   | 1       |         |         |         |         |        | 1      |
|    | 1     | 2           | 3        | 4          | 5       | 6       | 7       | 8       | 9       | 10      | 11      | 12     |        |
|    | 0     |             |          |            |         |         |         |         |         |         |         |        |        |
|    | 0     | 2.49869     | 2.51361  | 1.84246    | 2.05961 | 1.07906 | 0.18576 | 0.03507 | 0.0213  | 0.02312 | 0.02515 | 0      |        |
|    | 0     | 3.79014     | 4.68657  | 4.3493     | 4.07266 | 2.30186 | 0.38325 | 0.06629 | 0.02609 | 0.0246  | 0.02494 | 0      |        |
|    | 0     | 6.13374     | 4.48     | 4.65411    | 4.68857 | 2.40562 | 0.4515  | 0.06298 | 0.02762 | 0.02317 | 0.02425 | 0      |        |
|    | 0     | 1.76234     | 2.32573  | 2.3058     | 1.79709 | 1.12415 | 0.38487 | 0.06129 | 0.03142 | 0.02788 | 0.02856 | 0      |        |
|    | 0     | 1.96571     | 2.47976  | 2.45668    | 1.6681  | 0.75452 | 0.15193 | 0.03745 | 0.02267 | 0.02873 | 0.02725 | 0      |        |
|    | 0     | 5.23174     | 5.15026  | 3.98534    | 3.55127 | 2.31853 | 0.39086 | 0.05767 | 0.02572 | 0.02385 | 0.0224  | 0      |        |
|    | 0     | 4.46098     | 5.48986  | 4.53127    | 3.59156 | 2.24422 | 0.34404 | 0.06237 | 0.02686 | 0.0221  | 0.02628 | 0      |        |
|    | 0     | 1.78194     | 2.6407   | 1.83201    | 2.02373 | 1.1996  | 0.34977 | 0.06353 | 0.03068 | 0.02375 | 0.02658 | 0      |        |
|    |       |             |          |            |         |         |         |         |         |         |         |        |        |
|    |       |             |          |            |         |         |         |         |         |         |         |        |        |

- Once selected, the location on the right can be selected by a click-and-drag. These are both then under the same sample type.



### 3) DESIGN THE PLATE MAP

- ❑ The colour can also be changed by selecting the colour box:

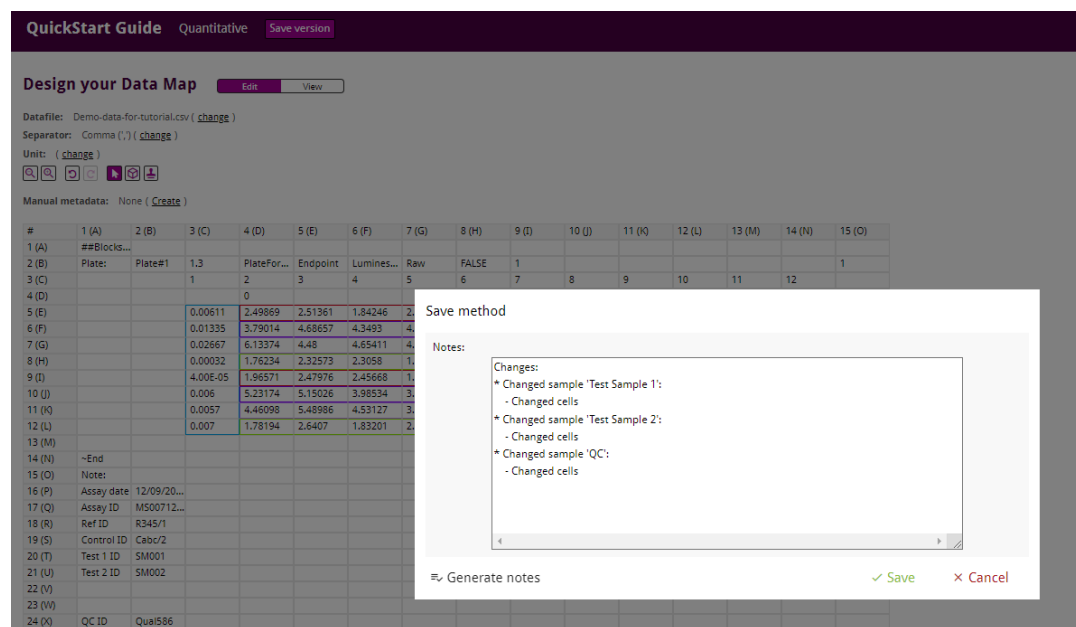


- ❑ Next, the same is repeated for locating the **reference**, **QC** and **test** samples.
- ❑ To save, the tick will apply these changes.
- ❑ To delete any samples, the bin icon will delete selected samples.



### 3) DESIGN YOUR DATA MAP

- This brings up a pop-up screen:



- Additional notes can be added manually before saving OR *Generate notes* can be selected and the changes made are automatically listed.



# 3) DESIGN YOUR DATA MAP

## Adding your doses

- ❑ Select the dilution icon when a sample is selected.
  - ❑ Use the “magic wand” tool and select the operation and steps necessary:
    - The Quick Start Guide data set uses the series shown to the left (start 25, step 2 division)
    - Complete as shown then click on the starting cell and drag to the end cell
- \*If, in practise, the doses are not a series, select enter dose instead of the magic wand to input manually.*
- ❑ Repeat with the other samples, except for the control wells which have a dose of 0.
  - ❑ When finished, click *Save Version* at the top of the page.



What is this called?

Reference

What is it?

Reference



Dilution



Start from: 25

Step by: 2

|          |         |         |         |         |         |         |          |           |             |             |         |
|----------|---------|---------|---------|---------|---------|---------|----------|-----------|-------------|-------------|---------|
|          | 0       |         |         |         |         |         |          |           |             |             |         |
| 0.00611  | 25      | 12.5    | 6.25    | 3.125   | 1.5625  | 0.78125 | 0.390625 | 0.1953125 | 0.097656... | 0.048828... | 0.01103 |
| 0.01335  | 3.79014 | 4.68657 | 4.3493  | 4.07266 | 2.30186 | 0.38325 | 0.06629  | 0.02609   | 0.0246      | 0.02494     | 0.00538 |
| 0.02667  | 6.13374 | 4.48    | 4.65411 | 4.68857 | 2.40562 | 0.4515  | 0.06298  | 0.02762   | 0.02317     | 0.02425     | 0.02206 |
| 0.00032  | 1.76234 | 2.32573 | 2.3058  | 1.79709 | 1.12415 | 0.38487 | 0.06129  | 0.03142   | 0.02788     | 0.02856     | 0.0027  |
| 4.00E-05 | 25      | 0       | 0       | 0       | 0       | 0       | 0        | 0         | 0           | 0           | 0.00186 |
| 0.006    | 5.23174 | 5.15026 | 3.98534 | 3.55127 | 2.31853 | 0.39086 | 0.05767  | 0.02572   | 0.02385     | 0.0224      | 0.00505 |
| 0.0057   | 4.46098 | 5.48986 | 4.53127 | 3.59156 | 2.24422 | 0.34404 | 0.06237  | 0.02686   | 0.0221      | 0.02628     | 0.02537 |
| 0.007    | 1.78194 | 2.6407  | 1.83201 | 2.02373 | 1.1996  | 0.34977 | 0.06353  | 0.03068   | 0.02375     | 0.02658     | 0.02928 |



# 3) DESIGN YOUR DATA MAP

## Incorporating metadata


- ❑ Metadata are field labels that will be populated from the imported values of each plate's dataset. Think of them as the label on a box, into which will be put the ID information read from imported data files.
  - There is metadata related to samples (sample identifiers) and metadata related to the method (e.g. assay date, operator, reagent ID, etc).
- ❑ Using the metadata icon, the cell holding this information is selected and a pop-up emerges at the top of the page.
- ❑ The suggested fields and completed and saved very similar to locating samples done earlier.



- Add metadata to the 9 items listed below

|            |             |   |
|------------|-------------|---|
| ~End       |             |   |
| Note:      |             |   |
| Assay date | 12/09/20... | 1 |
| Assay ID   | MS00712...  | 2 |
| Ref ID     | R345/1      | 3 |
| Control ID | Cabc/2      | 4 |
| Test 1 ID  | SM001       | 5 |
| Test 2 ID  | SM002       | 6 |
|            |             |   |
|            |             |   |
| QC ID      | Qual586     | 7 |
| ~End       |             |   |
| Note:      |             |   |
| Operator   | Ian         | 8 |
| Reagent ID | Lot20Jun    | 9 |

- To create new labels:

- Click: 
- Select the cell with the data
- Enter the *name*
- Select *What is it? (Sample Identifier or Metadata)*:
  - **Sample Identifier** refers to the key items on the plate
    - Reference
    - Test
    - Control
    - QC
  - **Metadata** refers to any other information e.g. operator ID, critical reagent lot number etc.
- *Select data type*
- Click the tick to save



## 4) ANALYSIS DEFINITION

- ❑ Select *Design your Analysis* (left side menu)
- ❑ Select the model *Type* you want to use.
  - 4PL for this dataset
- ❑ Under *Transform response*:
  - This dataset needs a  $\log_{10}$  response transformation
- ❑ Select other suitability criteria (or leave as default for now)

Design your Analysis

**1 Run your calculation** Quick fit Full Analysis

**Analysis Definition**

Model  
Linear Model FourPL Model FivePL Model

Prior Dose Transformation? None Log<sub>2</sub> Log<sub>e</sub> Log<sub>10</sub>

Combined Report? ☐

Transform Dose? Log<sub>10</sub>

Transform Response? Log<sub>10</sub>

Outlier Identification? None Log<sub>2</sub> Log<sub>e</sub> Log<sub>10</sub>

Use Weights? Square root Squared (c<sub>1</sub> x response) + c<sub>2</sub>

Variance Estimation Method? Residuals Lack of Fit Pure Error

B is Positive? ☒

Method For Ratios? Delta Method Feller's Theorem

+ Control Wells

+ Reference

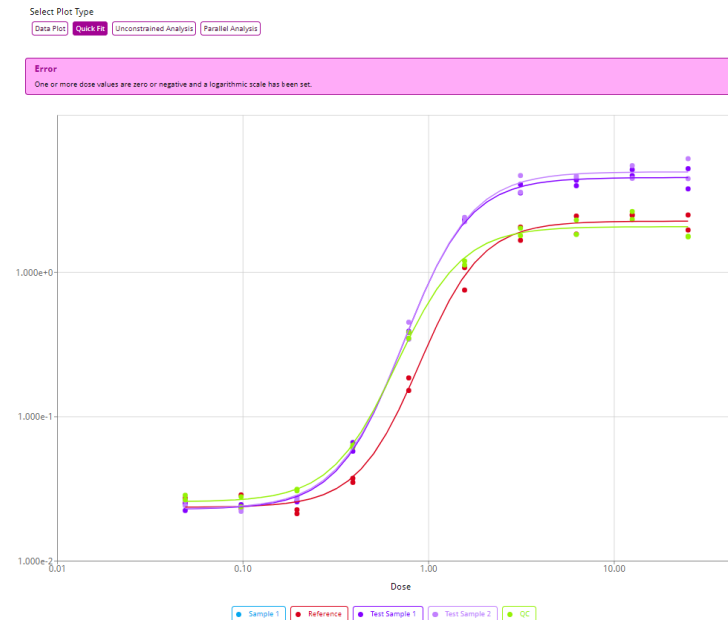
+ Quality Control

+ Sample Suitability



## 4) ANALYSIS DEFINITION – Quick Fit Analysis

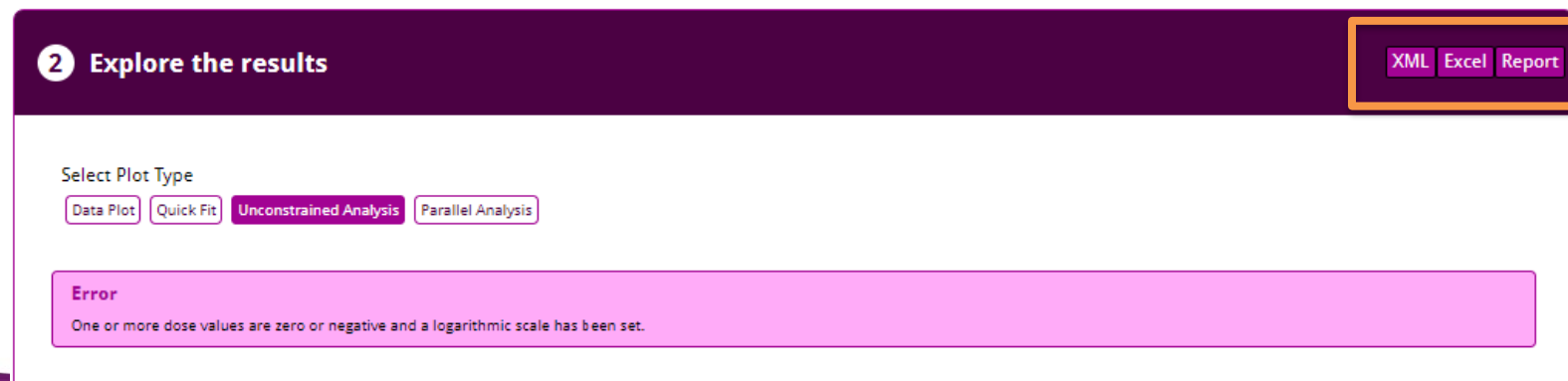
- ❑ For a quick view of your results and for an instant plot, select the *Quick Fit* option by 'Run your Calculation'.
- ❑ This will run a few second analysis before showing a plot under the 'Quick Fit' tab on the right.





## 4) ANALYSIS DEFINITION – Quick Fit Analysis

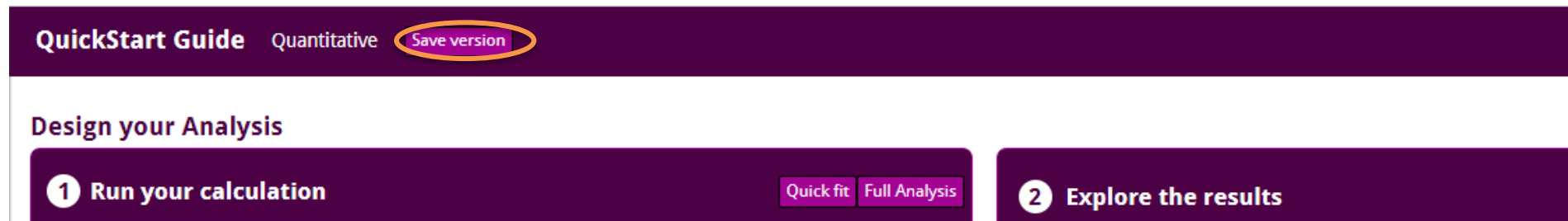
- For a full analysis that produces results and reports, select *Full Analysis* by 'Run your Calculation' with the same analysis definitions as before.
- This will run a full analysis which may take a few minutes.
  - This takes slightly longer as QuBAS demonstrates Diverse Self-Checking Programming Pairs (DSCPP) using two different branches. If you want to learn more, head on over to this link: <https://www.quantics.co.uk/qubas-bioassay-software/crtv-explained/>.





## 4) ANALYSIS DEFINITION – Quick Fit Analysis

- Once run, the report options pop up on the top right.
- Clicking *Report*, automatically downloads a PDF report which includes all the figures, relative potency results and suitability criteria which may have been added.
- Don't forget to *Save version* every time changes are made and or an analysis is run.





# Statistical Analysis Report

## Method: QuickStart Guide

### 1 Assay Details

| Substance ID  | Type                   |
|---------------|------------------------|
| Reference     | Reference Standard     |
| QC            | Quality Control Sample |
| Sample 1      | Test Sample            |
| Test Sample 1 | Test Sample            |
| Test Sample 2 | Test Sample            |

Table 1: Assay samples

| Name       | Content           |
|------------|-------------------|
| Assay Date | 12 September 2018 |

Table 2: Metadata

### 2 Summary

| System Suitability | Test Sample   | Sample Suitability | Relative Potency | 95% Confidence Interval |             |
|--------------------|---------------|--------------------|------------------|-------------------------|-------------|
|                    |               |                    |                  | Lower Limit             | Upper Limit |
| PASS               | Sample 1      | FAIL               | No result        | No result               | No result   |
|                    | Test Sample 1 | PASS               | 1.446            | 1.260                   | 1.658       |
|                    | Test Sample 2 | PASS               | 1.465            | 1.259                   | 1.704       |

Table 3: Summary of results

### 3 Analysis Details

Analysis type: Four Parameter Logistic Model (4PL)  
 Sign of slope parameter: Positive  
 Dose transformation in original data: None  
 Dose transformation in software:  $\log_{10}$   
 Response transformation in software:  $\log_{10}$   
 Variance estimate: Calculated using residuals  
 Confidence intervals of ratios: Calculated using the delta method

### 7 Test Sample: Test Sample 1

| Name          | Dose  | Geometric Mean Response | %GCV of Response |
|---------------|-------|-------------------------|------------------|
| Test Sample 1 | 0.05  | 0.024                   | 7.89             |
| Test Sample 1 | 0.10  | 0.024                   | 2.21             |
| Test Sample 1 | 0.20  | 0.026                   | 1.02             |
| Test Sample 1 | 0.39  | 0.062                   | 10.35            |
| Test Sample 1 | 0.78  | 0.387                   | 1.40             |
| Test Sample 1 | 1.56  | 2.310                   | 0.51             |
| Test Sample 1 | 3.13  | 3.803                   | 10.17            |
| Test Sample 1 | 6.25  | 4.163                   | 6.37             |
| Test Sample 1 | 12.50 | 4.913                   | 6.90             |
| Test Sample 1 | 25.00 | 4.453                   | 25.60            |

GCV = Geometric Coefficient of Variation

Table 10: Summary of Test Sample 1

#### 7.1 Model fits

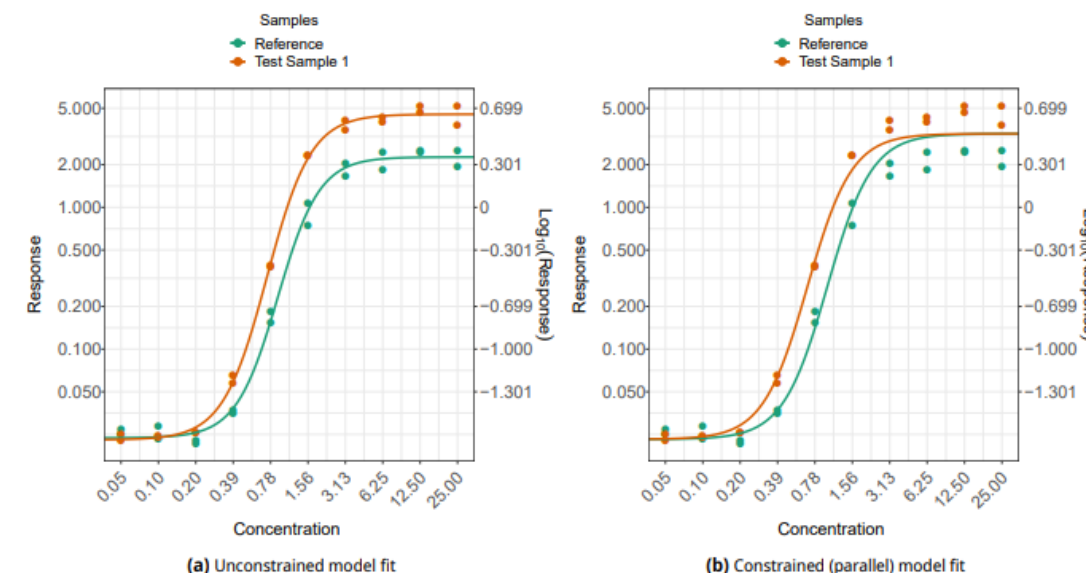


Figure 4: Model fits to Reference and Test Sample 1





#### DATA MAP

- Data Files
- Design your Data Map

#### ANALYSIS

- Manage your Metadata
- Design your Analysis

#### SIGN OFF

- Method Version History
- Submit for Sign Off

## QuickStart Guide

### Design your Analysis

#### 1 Run your Analysis

#### Analysis Design

##### Model

Linear Model Four

##### Prior Dose Transformation

None Log<sub>10</sub> Log<sub>e</sub>

Method Version History ?

Transform Dose?

Transform Responses

Outlier Identification

Use Weights?

#### QuickStart Guide Quantitative Save version

#### Method Version History

| Date                   | History | Default version   | Changes by                     | Data file                  | Analysis |
|------------------------|---------|---|--------------------------------|----------------------------|----------|
| JUNE 2022              |         |   |                                |                            |          |
| 23 June 2022, 08:35:46 |         | <input type="radio"/>                                   | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 23 June 2022, 08:35:46 |         | <input type="radio"/> Current                           | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv | ✓        |
| 23 June 2022, 08:35:15 |         | <input type="radio"/>                                   | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 23 June 2022, 08:34:38 |         | <input type="radio"/>                                   | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 23 June 2022, 08:34:08 |         | <input checked="" type="radio"/>                        | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 23 June 2022, 08:32:53 |         | <input type="radio"/> <a href="#">Open this version</a> | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 22 June 2022, 11:05:19 |         | <input type="radio"/>                                   | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 22 June 2022, 11:01:02 |         | <input type="radio"/>                                   | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 22 June 2022, 10:54:56 |         | <input type="radio"/>                                   | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 22 June 2022, 10:54:34 |         | <input type="radio"/>                                   | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 22 June 2022, 10:33:30 |         | <input type="radio"/>                                   | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |
| 22 June 2022, 09:58:50 |         | <input type="radio"/>                                   | eleanor.harriss@quantics.co.uk | Demo-data-for-tutorial.csv |          |



# THE METHOD VERSION HISTORY

- ❑ All versions of the method saved will be recorded here, with the date, notes generated and which version is currently being used.
- ❑ If you hover over the versions, a path demonstrating the saved version journey and its parent versions.
- ❑ Previous versions can be re-visited when **Open this version** is selected.



THE FOLLOWING 6 PAGES COVER THE 3 STEPS SHOWN ABOVE  
REQUIRED TO **LOCK A METHOD FOR ROUTINE (GMP) USE**



# LOCK THE METHOD FOR ROUTINE (GMP) USE

1) Submit as MCF\*

- In **DEVELOPMENT MODE** – Development Record, submit the Method for sign off. \*MCF (method configuration file)

2) Set Auto Import folder (OPTIONAL)

- Set up the folder that QuBAS will “watch” for automatic import of data files

3) Sign off the Method for GMP use. First signature\*



- In **ROUTINE MODE** as Sign off user: Sign off Method for Routine (GMP) use.

\* System can be set to require 2 different signatures if required









## DATA MAP

-  Data Files
-  Design your Data Map

## ANALYSIS

-  Manage your Metadata
-  Design your Analysis

## SIGN OFF

-  Method Version History
-  Submit for Sign Off

## QuickStart Guide Quantitative

## Submit for Sign Off

New submission

[Prepare attachments](#)Auto Import ☐Auto Export PDF ☐Auto Export XML ☐

Auto Import Path



Notes

[Submit for Sign Off](#)



# SUBMIT FOR SIGN OFF

- ❑ All analyses saved for the recently run method will be shown when *Prepare attachments* is clicked.



- ❑ When ready to lock the setup for Routine (GMP) :
  - Do one final analysis of a trial dataset with ALL analysis options required
  - Save this version and check the report
  - Add notes before you click *Submit*
- ❑ The screen will then demonstrate that this method is awaiting approval.



## QuickStart Guide Quantitative

### Submit for Sign Off

New submission

Prepare attachments

Auto  
Import



Auto Export  
PDF



Auto Export  
XML



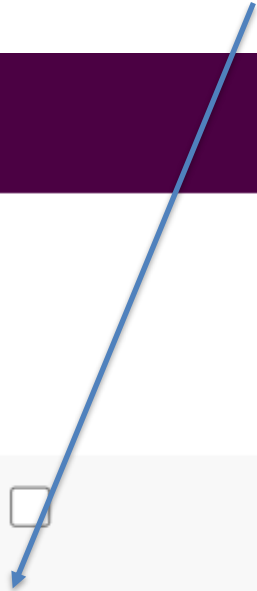
Auto Import Path



Notes

Notes

Copy address as text





# SETTING AUTO IMPORT FOLDER

- ❑ QuBAS can be set to “watch” a pre-specified folder for a new data file to analyse. When a file appears, QuBAS imports it and runs the analysis automatically.
- ❑ To use Auto Import QuBAS must have access to that folder. On a network, this may require your IT Admin to create a suitable folder.
  - ❑ More information is available in the installation guide. If you are testing QuBAS on a virtual server this won't be possible.
- ❑ If required, set the location of this folder (specific to this Method) here
  - Use Windows file explorer to browse to the Folder location
  - Right click on address bar and *Copy address as text*
  - Paste into pop up box



Sign Off

MCF Version 1

| > | Date             | Data Map    | Analysis Definition | Template     | Plugin Used | Auto Import Folder Location | User Notes       |
|---|------------------|-------------|---------------------|--------------|-------------|-----------------------------|------------------|
|   | 02 December 2019 | Version - 2 | Version - 2         | New Template | N/A         | N/A                         | Submitted as MCF |

1

Approve for Audit 1?


Notes

Confirm Cancel

2



# SIGN OFF A METHOD FOR ROUTINE USE

- ❑ Log in to **ROUTINE MODE** as a user with Sign Off permissions
- ❑ Select the method that you wish to sign off
- ❑ Select Sign off Tab in top menu
- ❑ The locked method is shown. Click  to download a report of the Method parameters if required. ①
- ❑ Add suitable note and click *Confirm* to sign off the Method. ②
  - If dual sign off has been selected by your Administrator, this will then be sent to the Audit room for the second sign off. If you don't have a second audit sign off, this button will just be 'Approve' and will now be available for Routine use.



# QUBAS ROUTINE (RELATIVE POTENCY) **GMP MODE**



The steps shown here are required to run a Routine Relative Potency analysis.

*1a) Manual*

*1b) Automated*

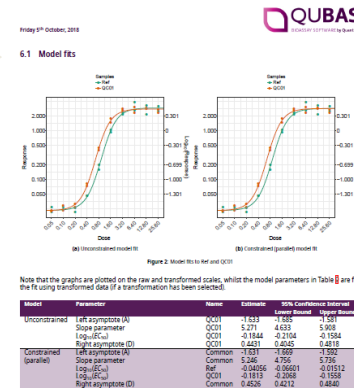
1a) Import data sets manually

2) Create a batch of 1 or more files to analyse

3) Start analysis run

1b) Automatically save data file(s) to auto import folder

Export Report







## License

Please select required mode of operation

Explore Mode

Routine Mode

Audit and second sign-off access

Admin

0/10

Licences in use

4310

RP Tokens Remaining

9616

IA Tokens Remaining

## Log in

Please enter your account credentials

Email

ian.yellowlees@quantics.co.uk

Password

••••••••

0

1

2

3

4

5

6

7

8

9

PIN

•••••



[Change Credentials](#)

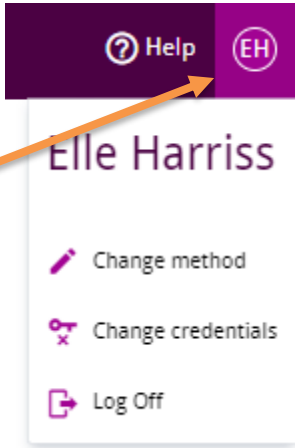
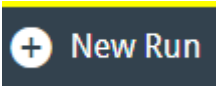
Log in





# USING ROUTINE MODE

## Manual data file import

- ❑ Log in as Routine user (you may need to log out first - click  )
- ❑ Select the same Method in Routine mode.
- ❑ Import a data file (described earlier for Explore Mode; pg10-12).
- ❑ Select Routine from the top menu
  - This will display a screen of all the routine analyses that have been run for this Method.
  - Routine mode analyses files in batches of 1 or more called “Runs”
- ❑ Click 
- ❑ Select files for analysis. Click *Next, Next, Continue.*

 *Only files that have not previously been run are available.*



## Run Report Setup

Configure report parameters

Demo Routine run

1

### MetaData

2

Select All

Select None

☒ AssayID

☒ Reagent

☒ Assay Date

☒ Operator ID

Demo Routine run

Update Run ↗

3



- 1) Give the Run a name ①
- 2) Select which Metadata you wish to be in the report ②
- 3) Click *Update run* ③

Click *Start Run*

..... *When complete Download Report (bottom right)*



# THE MONITORING ROOM

- ❑ All analyses saved in the Development mode, and all Routine analyses are automatically saved to the Monitoring room.
  - Click the top right *Monitoring* tab
  - Please note with a new Method there will only be one analysis until more data sets are run
- ❑ Explore the data!
  - **Filter <** the datasets in the output by any Metadata, Analysis Definition, Data Map Version, MCF Version, Run Date Range & Run Type
  - x axis / y axis options should be straight forward.
- ❑ You can hover over a data points to show its details and download its report (download is for Routine mode reports only).



Filter >

Select All Select None

Type: Explore  
Report ID: 502  
Filename: file10LIYD.csv  
Run Date: 05/Oct/2018

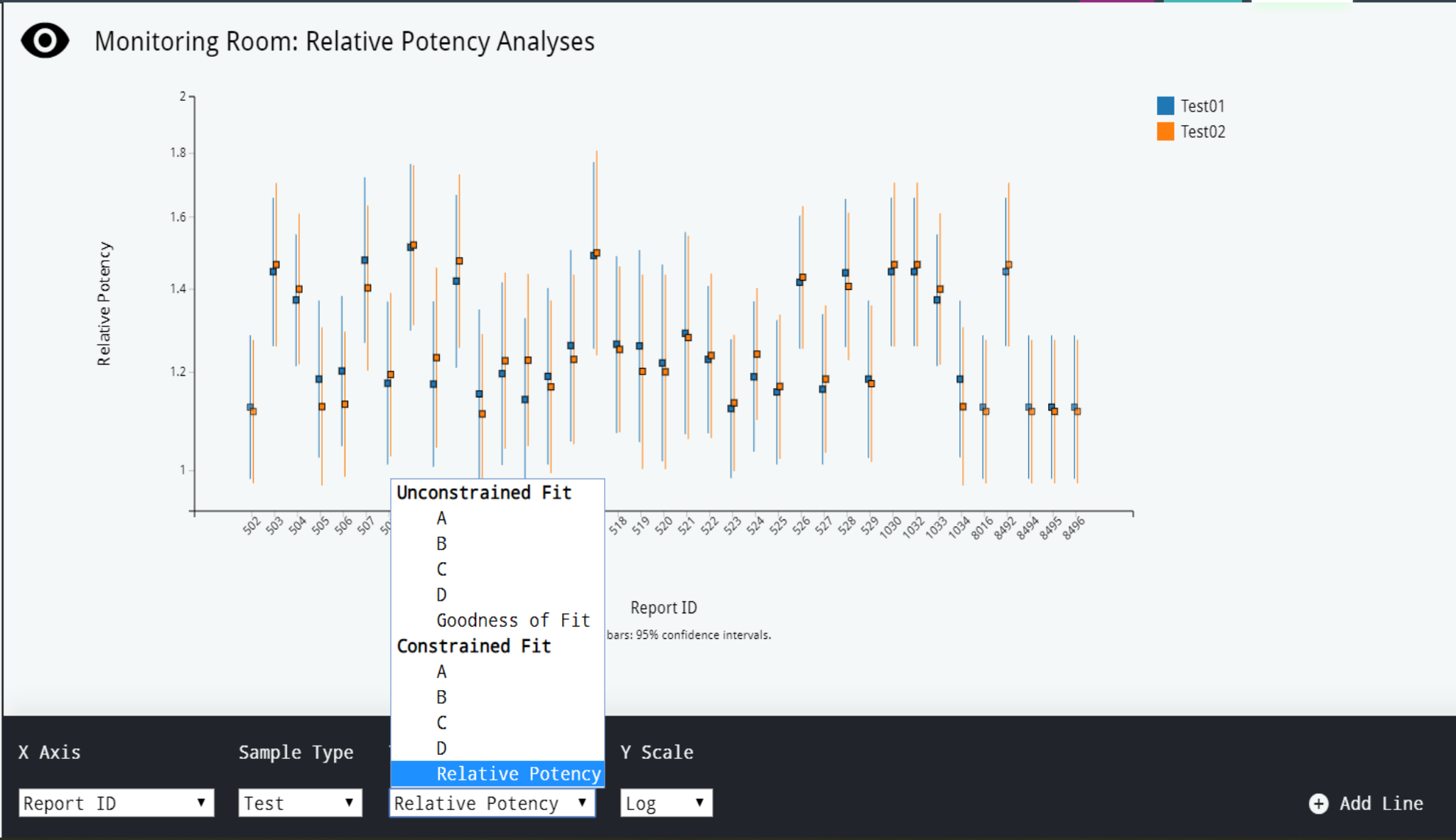
Type: Routine  
Run: AutoImport-05/Oct/1  
Report ID: 503  
Filename: file10JEVTM.cs  
Run Date: 05/Oct/2018

Type: Routine  
Run: AutoImport-05/Oct/1  
Report ID: 504  
Filename: file110JFRH.cs  
Run Date: 05/Oct/2018

Type: Routine  
Run: AutoImport-05/Oct/1  
Report ID: 505  
Filename: file12FTHZJ.cs  
Run Date: 05/Oct/2018

Type: Routine  
Run: AutoImport-05/Oct/1  
Report ID: 506  
Filename: file13SXWDK.cs  
Run Date: 05/Oct/2018

Type: Routine  
Run: AutoImport-05/Oct/1





# QuBAS INTERPOLATION ANALYSIS (IA)

...using the Bursa-Yellowlees mathematically  
efficient methodology





## Create New Method

IA EH

☐ Quantitative

☐ Quantal

☒ Interpolation Analysis

Cancel ✕

Save ✓



⚠ QuBAS IA functions are the same as for Relative potency analysis with the following exceptions:

- QuBAS IA can create automatically labelled test samples
- Sample suitability criteria are different.

□ Create an IA Method as shown above (please refer to the RP introduction as a reminder of how to create a method p8 - 9 )

- Add Name



## Design your Data Map

Edit

View

**Datafile:** Demo-data-for-Interpolation.csv ( [change](#) )

**Separator:** Comma (',' ) ( change )

Unit: ( change )Manual metadata: None ( [Create](#) )[illegible]



- Set up the Data Map as for RP (p13 -22). This Demo data set has
  - 1 Standard sample (reference)
  - 1 dose response QC sample
  - 24 test samples – The demo will use automatic sample labelling.
  
- The location of metadata items in the data file are added in the same way as in an RP analysis



# DESIGN THE PLATE MAP

❑ Assign the Standard (Reference) and Named QC samples to the Plate Map to replicate the image above.

❑ Add the dilution information below using the magic wand for the doses: 

❑ **Standard** = Division, Start 0.9, Step 3

❑ **QC** = Multiplication, Start 1, Step 3

❑ To create Automatic samples

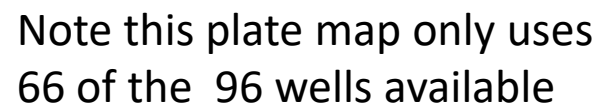
- Select Automatic Test Sample under *What is it?*
- Drag to create the first automatic sample
- Add the dilution information

Test = Multiplication, Start 1, Step 3




|                    |             |             |             |             |            |
|--------------------|-------------|-------------|-------------|-------------|------------|
| Value: 0.863077152 |             |             |             |             | 6 (F)      |
| 54...              | 1.959751... | 1/1         | 1/3         | 1.384554... | 0.57598... |
| 56...              | 1.145347... | 0.896352... | 0.323150... | 1.116916... | 0.43772... |

**Automatic Test Sample 1** Automatic Test Sample  
Dose/Dilution: 1  
Value: 0.863077152

[illegible]



- ❑ 1) Select the Stamp tool  and select the initial sample to copy
- ❑ 2) Then outline the whole area (including initial sample) to paste the new automatic samples
  - Repeat as required
- ❑ 3) Samples are created and labelled. You can now *Save Version*.



The remaining screens for IA are similar to RP analysis with some differences in sample suitability criteria and analysis options - please see p23 - 29

Monitoring room for IA analysis will be available in later versions of QuBAS