

# Package ‘OAtools’

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**Title** Analysis of OpenArray PCR Data

**Version** 1.0.0

**Description** Provides a suite of R functions to analyze gene expression experiments on the OpenArray real-time PCR platform. OAtools fits logistic regressions to fluorescence curves to distinguish between real amplification and false positives. OAtools supports data import, analysis, and visualization through plots and a dynamic HTML report.

**License** GPL (>= 3)

**LazyData** FALSE

**Depends** R (>= 4.6)

**Imports** basilisk (>= 1.20.0), Biobase (>= 2.70.0), dplyr (>= 1.1.4), DT (>= 0.34.0), ggplot2 (>= 3.5.2), janitor (>= 2.2.1), methods (>= 4.5.2), plotly (>= 4.11.0), purrr (>= 1.2.0), ReadqPCR (>= 1.56.0), readxl (>= 1.4.5), reticulate (>= 1.43.0), rlang (>= 1.1.6), rmarkdown (>= 2.29), S4Vectors (>= 0.48.0), shiny (>= 1.13.0), SummarizedExperiment (>= 1.40.0), tibble (>= 3.3.0), tidyr (>= 1.3.1), writexl (>= 1.5.4)

**Suggests** testthat (>= 3.0.0), knitr, kableExtra (>= 1.4.0), NormqPCR (>= 1.56.0), BiocManager (>= 1.30.27)

**biocViews** qPCR, GeneExpression, DataImport, Regression

**BugReports** <https://github.com/uwvirology-ngs/OAtools/issues>

**URL** <https://github.com/uwvirology-ngs/OAtools>

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---

*.buildServer*                      *Web Server*

---

**Description**

Helper method to `buildApp()` responsible for construction of the Shiny web server

**Usage**

```
.buildServer(input, output, session)
```

**Arguments**

<code>input</code>	reactive values from UI widgets
<code>output</code>	render functions for results
<code>session</code>	environment for user session

**Value**

A Shiny web server

---

*.buildUI*                              *User Interface*

---

**Description**

Helper method to `buildApp()` responsible for construction of the graphical user interface

**Usage**

```
.buildUI()
```

**Value**

A Shiny UI

---

`.runFitCurve`                      *Run the fit\_curve() function*

---

### Description

A thin R wrapper for the python3 function `fit_curve()`, which attempts to optimize 5-parameter logistic regressions to PCR fluorescence curves.

### Usage

```
.runFitCurve(pcr_data, linear_threshold)
```

### Arguments

<code>pcr_data</code>	A data.frame with the following required columns: <b>cycle</b> PCR cycle number <b>fluo</b> observed fluorescence
<code>linear_threshold</code>	numeric value specifying the minimum overall change-in-fluorescence over the PCR reaction required for the optimizer to attempt fitting a logistic model

### Value

The model as a nested list

---

`.serverDataImport`                      *Data Import Server*

---

### Description

Data Import Server

### Usage

```
.serverDataImport(id)
```

### Arguments

<code>id</code>	identifier unique to Data Import page
-----------------	---------------------------------------

### Value

The Data Import server component

---

.serverFitCurves      *Curve Fitting Server*

---

**Description**

Curve Fitting Server

**Usage**

.serverFitCurves(id, se)

**Arguments**

id	identifier unique to Fit Curves page
se	SummarizedExperiment with OpenArray assay data

**Value**

The Fit Curves server component

---

.serverGraphics      *Graphics Server*

---

**Description**

Graphics Server

**Usage**

.serverGraphics(id, se)

**Arguments**

id	identifier unique to Graphics page
se	SummarizedExperiment with OpenArray assay data

**Value**

The Graphics server component

---

`.serverReporting`      *Reporting Server*

---

**Description**

Reporting Server

**Usage**

```
.serverReporting(id, se_fit)
```

**Arguments**

<code>id</code>	identifier unique to Reporting page
<code>se_fit</code>	SummarizedExperiment with OpenArray assay data

**Value**

The Reporting server component

---

`.uiDataImport`      *Data Import UI*

---

**Description**

Data Import UI

**Usage**

```
.uiDataImport(id)
```

**Arguments**

<code>id</code>	identifier unique to Data Import page
-----------------	---------------------------------------

**Value**

The Data Import page

---

.uiFitCurves                      *Curve Fitting UI*

---

**Description**

Curve Fitting UI

**Usage**

.uiFitCurves(id)

**Arguments**

id                      identifier unique to Fit Curves page

**Value**

The Fit Curves page

---

.uiGraphics                      *Graphics UI*

---

**Description**

Graphics UI

**Usage**

.uiGraphics(id)

**Arguments**

id                      identifier unique to Graphics page

**Value**

The Graphics page

---

`.uiReporting`*Reporting UI*

---

**Description**

Reporting UI

**Usage**`.uiReporting(id)`**Arguments**`id` identifier unique to Reporting page**Value**The Reporting page

---

`buildApp`*A Shiny App for OAtools*

---

**Description**

Builds a Shiny application for interactively running OAtools

**Usage**`buildApp()`**Details**

Temporarily changes the maximum file size for upload to 30MB, restoring the original setting upon application exit.

**Value**

A Shiny web application

**Examples**`app <- buildApp()`

---

`computeModels`*Optimize SPL models to OpenArray PCR data and save as metadata*

---

## Description

Computes 5-parameter logistic models optimized to PCR data contained in the specified assay matrix, either `fluo_normalized` or `fluo_reporter`. The former refers to the base-line adjusted, normalized fluorescence from the Amplification Data tab of the original Excel output. The latter refers to the multicomponent fluorescence from the Multicomponent Data tab.

The expected input for this function is a `SummarizedExperiment` object containing OpenArray PCR data, which can be generated by calling the `excelToSE()` function of the package on the raw Excel output from QuantStudio software.

## Usage

```
computeModels(se, assay_name, linear_threshold = 400)
```

## Arguments

<code>se</code>	OpenArray PCR data as a <code>SummarizedExperiment</code> object
<code>assay_name</code>	character value specifying the assay matrix from which to load PCR data for curve-fitting, either <code>fluo_normalized</code> or <code>fluo_reporter</code>
<code>linear_threshold</code>	numeric value specifying the minimum overall change-in-fluorescence over the PCR reaction required for the optimizer to attempt fitting a logistic model

## Details

Under the hood, this function invokes `.runFitCurve()`, a thin wrapper which calls python3 code to fit models with `scipy.optimize`, on each PCR reaction of the OpenArray plate separately. The computed models are added to the `SummarizedExperiment` container in metadata, named as `assay_name + _models`. For example, `fluo_normalized_models` would be created in the experiment metadata if `computeModels(assay_name = "fluo_normalized")` is called.

## Value

OpenArray PCR data as a `SummarizedExperiment` object with information from the computed model stored as metadata.

## Examples

```
path <- system.file(  
  "extdata",  
  "oa_gene_expression_1.xlsx",  
  package = "OAtools"  
)
```

```
se <- excelToSE(excel_path = path) |>
  computeModels(assay_name = "fluo_normalized") |>
  computeModels(assay_name = "fluo_reporter")
```

---

determinePCRResults *Determine PCR results from fit curves*

---

## Description

Assigns positive or negative PCR results to each reaction depending on the equation of the model optimized to observed multicomponent fluorescence values. The reporter dye fluorescence without normalization is used to distinguish between real amplification and false positives.

## Usage

```
determinePCRResults(se, key_path)
```

## Arguments

se	a SummarizedExperiment object containing OpenArray qPCR Data
key_path	file path to the target-threshold key

## Details

The key is an Excel file storing values used by determinePCRResults() to categorize PCR curves as positive or negative. In the key, each gene is associated with threshold values for Crt, change-in-fluorescence, and slope at the reaction midpoint.

For more specifics, input ?target\_threshold\_key into the R console.

## Value

a SummarizedExperiment

## Examples

```
data(example_se)

key_path = system.file(
  "extdata",
  "target_threshold_key.xlsx",
  package = "OAtools"
)

se <- example_se |>
  determinePCRResults(key_path = key_path)
```

---

`example_se`*Example OpenArray Gene Expression Data Contained in a SummarizedExperiment*

---

### Description

A sample of OpenArray gene expression data from respiratory tract microbiota profiling experiments conducted at the UW Virology research lab on human nasal swabs. This file (.rda) stores the PCR data in a SummarizedExperiment container and is intended for use with package examples and unit testing.

### Format

a SummarizedExperiment object with the following:

**colData** information associated with each PCR well

**rowData** cycle numbers

**assays** matrices of fluorescence values by PCR well and cycle

### Details

Load this object into the environment with: `data(example_se)`

### Source

This object contains PCR data imported from the initial Excel QuantStudio output. Logistic and linear models were fit to the PCR data and stored as metadata.

The object can be reproduced from the package example data by running the following commands in the R console:

```
path <- system.file(
  "extdata",
  "oa_gene_expression_1.xlsx",
  package = "OAtools"
)

se <- excelToSE(excel_path = path) |>
  computeModels(assay_name = "fluo_normalized") |>
  computeModels(assay_name = "fluo_reporter")
```

---

`excelToSE`*Convert OpenArray data from Excel to a Summarized Experiment*

---

**Description**

Transforms raw gene expression run data exported from the OpenArray QuantStudio 12K Flex Software from .xlsx format into an instance of the SummarizedExperiment class from Bioconductor.

**Usage**

```
excelToSE(excel_path, header_rows = 17, skip = 19)
```

**Arguments**

<code>excel_path</code>	file path to the Excel document containing the PCR data
<code>header_rows</code>	number of rows of run metadata to read in from the header
<code>skip</code>	number of rows to skip when reading fluorescence data or results

**Value**

OpenArray PCR data as a SummarizedExperiment object

**Examples**

```
path = system.file(  
  "extdata",  
  "oa_gene_expression_1.xlsx",  
  package = "OAtools"  
)  
  
se <- excelToSE(excel_path = path)
```

---

`generateReport`*Generate a PCR Report*

---

**Description**

Knits an HTML report summarizing the OpenArray experiment and saves to the specified directory.

**Usage**

```
generateReport(se, path = tempdir(), model_results = FALSE)
```

**Arguments**

se	a SummarizedExperiment containing OpenArray qPCR data
path	intended outfile path, defaults to a temporary directory
model_results	boolean value indicating whether to include the results column, which is created when deriving results using the curve-fitting method

**Value**

An HTML Report summarizing the OpenArray experiment

**Examples**

```
data(example_se)
generateReport(se = example_se)
```

---

oa\_gene\_expression\_1 *Example Raw OpenArray Gene Expression Data*

---

**Description**

The first of two Excel files storing run data from separate OpenArray gene expression experiments. The context behind the experiment was respiratory tract microbiota profiling on human nasopharyngeal swabs from patients experiencing respiratory syndromes.

**Format**

An Excel file (.xlsx) with three tabs:

**Amplification Data** normalized fluorescence by cycle number

**Multicomponent Data** spectral contribution of the reporter dye by cycle number

**Results** PCR results, PCR well metadata, and QC metrics

**Details**

Access this file with: `system.file("extdata", "oa_gene_expression_1.xlsx", package = "OAtools")`

**Source**

This file was exported from QuantStudio 12K Flex Software after a gene expression run, then filtered down to include 12 samples and 4 genes for file size concerns.

---

oa\_gene\_expression\_2 *Example Raw OpenArray Gene Expression Data*

---

### Description

The second of two Excel files storing run data from separate OpenArray gene expression experiments. The context behind the experiment was respiratory tract microbiota profiling on human nasopharyngeal swabs on patients experiencing respiratory syndromes.

### Format

An Excel file (.xlsx) with three tabs:

**Amplification Data** normalized fluorescence by cycle number

**Multicomponent Data** spectral contribution of the reporter dye by cycle number

**Results** PCR results, sample metadata, and QC metrics

### Details

Access this file with: `system.file("extdata", "oa_gene_expression_2.xlsx", package = "OAtools")`

### Source

This file was exported from QuantStudio 12K Flex Software after a gene expression run, then filtered down to include 12 samples and 4 genes for file size concerns.

---

plotCrt *Plot Relative Cycle Threshold Values by Gene*

---

### Description

Generates a box and whisker plot visualizing the distribution of Crt values measured on an OpenArray plate by Gene.

### Usage

```
plotCrt(se)
```

### Arguments

se a SummarizedExperiment object containing OpenArray qPCR data

### Value

a ggplot2 figure

**Examples**

```
data(example_se)

plotCrt(example_se)
```

---

`plotModel`*Plot Fluorescence Values Predicted by Model*

---

**Description**

Juxtaposes the fluorescence values predicted by the model optimized to the measured fluorescence vs. cycle data for a particular well.

**Usage**

```
plotModel(
  se,
  well_id,
  assay_name,
  include_mdpt_tangent = FALSE,
  include_coldata_annotation = FALSE
)
```

**Arguments**

<code>se</code>	a SummarizedExperiment object containing OpenArray qPCR data
<code>well_id</code>	a character representing the name of the well to plot as listed in the assay matrix
<code>assay_name</code>	name for the assay matrix from which to pull observed fluorescence values, either <code>fluo_reporter</code> or <code>fluo_normalized</code>
<code>include_mdpt_tangent</code>	boolean determines whether to annotate the midpoint of the reaction and draw a tangent line to the model curve at that point
<code>include_coldata_annotation</code>	boolean determines whether to annotate the coldata onto the top left of the plot.

**Value**

a ggplot2 figure

**Examples**

```
data(example_se)

plotModel(
  example_se,
  well_id = "well_2665",
  assay_name = "fluo_reporter",
```

```

    include_mdpt_tangent = TRUE,
    include_coldata_annotation = TRUE
  )

```

---

plotOverview

*Plot Amplification Status by Sample and Gene*


---

### Description

Generates an overview graphic summarizing qPCR results for each combination of sample and gene on an OpenArray experiment.

### Usage

```
plotOverview(se)
```

### Arguments

se a SummarizedExperiment object containing OpenArray qPCR data

### Value

a ggplot2 figure

### Examples

```

data(example_se)

plotOverview(example_se)

```

---

plotQC

*Plot a 3D Quality Control Graphic from a SummarizedExperiment*


---

### Description

Generates a 3-dimensional quality control plot comparing the amplification status to the crt, Cq conf, and amplification score metrics output by QuantStudio 12K Flex Software.

### Usage

```
plotQC(se)
```

### Arguments

se a SummarizedExperiment object containing OpenArray qPCR data

**Value**

a plotly figure

**Examples**

```
data(example_se)
plotQC(example_se)
```

---

seToQPCRBatch	<i>Convert to qPCRBatch Object</i>
---------------	------------------------------------

---

**Description**

Transforms OpenArray run data contained within the SummarizedExperiment container into a qPCRBatch object. This conversion allows for convenient gene expression analyses with the NormqPCR package.

**Usage**

```
seToQPCRBatch(se)
```

**Arguments**

se                    A SummarizedExperiment object with OpenArray run data

**Value**

a qPCRBatch object

**Examples**

```
path = system.file(
  "extdata",
  "oa_gene_expression_1.xlsx",
  package = "OAtools"
)

se <- excelToSE(excel_path = path)

qpcr <- seToQPCRBatch(se)
```

---

target\_threshold\_key *Target Threshold Key*

---

**Description**

This Excel file (.xlsx) contains a table associating each assay target contained in the example gene expression run data with thresholds values. This key is optionally used to aid in concurrently interpreting data including numerous targets with dissimilar behaviors.

**Format**

An Excel sheet (.xlsx) with four columns:

target the target assay ID

slope\_threshold minimum acceptable slope in the exponential phase for a positive result

delta\_threshold minimum acceptable overall change in fluorescence for a positive result

crt\_threshold maximum acceptable crt for a positive result

**Details**

The example key is stored in the `inst/extdata/` directory of the package. Access this file with: `system.file("extdata", "target_threshold_key.xlsx", package = "OAtools")`.

**Source**

Written manually for use with resulting functions.

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