

# dpcReport: the coolest tool ever

---

Michał Burdukiewicz<sup>1</sup>, Jim Huggett<sup>2</sup>, Alexandra Whale<sup>2</sup>, Piotr Sobczyk<sup>3</sup>,  
Paweł Mackiewicz<sup>1</sup>, Andrej-Nikolai Spiess<sup>3</sup>, Peter Schierack<sup>5</sup>, and Stefan  
Rödiger<sup>5</sup>

<sup>1</sup>University of Wrocław, Department of Genomics,

<sup>2</sup>Molecular and Cell Biology Team, LGC, Teddington, United Kingdom,

<sup>3</sup>Wrocław University of Science and Technology, Faculty of Pure and Applied  
Mathematics,

<sup>4</sup>University Medical Center Hamburg-Eppendorf, Hamburg, Germany,

<sup>5</sup>Brandenburg University of Technology Cottbus-Senftenberg, Institute of  
Biotechnology

dPCR software

Reproducibility

## dPCR software

---



# Reproducibility

---

Scientific software supports reproducibility, otherwise it is not scientific.

A report must contain enough information to allow the full reproduction of the conducted analysis.

## Table of Contents

- [dpcReport](#)
  - [Data summary table](#)
    - [Explanation](#)
  - [Data summary scatter charts](#)
    - [Scatter chart](#)
  - [Compare runs](#)
  - [Compare digital PCR experiments](#)
    - [The mean number of template molecules per partition](#)
- [R code](#)
- [R Session](#)

## dpcReport

Report generated on 2017-03-27 07:12:26 using [dpcR](#) R package.

Detected input file: 20130918\_Dilution\_log10.csv.

md5 checksum of the input file: 6bf3306199dd7af439d1c8acd08e23c1

**The input was modified manually in dpcReport application.**

File format: QX100.

## Data summary table

Run	Experiment name	Replicate ID	Assay	Method	$\lambda$	$\lambda$ (lower CI)	$\lambda$ (upper CI)	Concentration	Concentration (lower CI)	Concentration (upper CI)	k	n
ABS1.A09.gDNA + P 10 <sup>4</sup>	ABS1	A09.gDNA + P 10 <sup>4</sup>	ileS	dube	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.A09.gDNA + P 10 <sup>4</sup>	ABS1	A09.gDNA + P 10 <sup>4</sup>	ileS	bhat	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.B09.gDNA	ABS1	B09.gDNA	ileS	bhat	0.07	0.07	0.08	1171.87	0.08	0.09	1140	11688

# Date and time

## Table of Contents

- [dpcReport](#)
  - [Data summary table](#)
    - [Explanation](#)
  - [Data summary scatter charts](#)
    - [Scatter chart](#)
  - [Compare runs](#)
  - [Compare digital PCR experiments](#)
    - [The mean number of template molecules per partition](#)
- [R code](#)
- [R Session](#)

## dpcReport

Report generated on 2017-03-27 07:12:26 using [dpcR](#) R package.

Detected input file: 20130918\_Dilution\_log10.csv.

md5 checksum of the input file: 6bf3306199dd7af439d1c8acd08e23c1

**The input was modified manually in dpcReport application.**

File format: QX100.

## Data summary table

Run	Experiment name	Replicate ID	Assay	Method	$\lambda$	$\lambda$ (lower CI)	$\lambda$ (upper CI)	Concentration	Concentration (lower CI)	Concentration (upper CI)	k	n
ABS1.A09.gDNA + P 10 <sup>4</sup>	ABS1	A09.gDNA + P 10 <sup>4</sup>	ileS	dube	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.A09.gDNA + P 10 <sup>4</sup>	ABS1	A09.gDNA + P 10 <sup>4</sup>	ileS	bhat	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.B09.gDNA	ABS1	B09.gDNA	ileS	bhat	0.07	0.07	0.08	1171.87	0.11	0.12	1110	11000



# Input file name

## Table of Contents

- [dpcReport](#)
  - [Data summary table](#)
    - [Explanation](#)
  - [Data summary scatter charts](#)
    - [Scatter chart](#)
  - [Compare runs](#)
  - [Compare digital PCR experiments](#)
    - [The mean number of template molecules per partition](#)
- [R code](#)
- [R Session](#)

## dpcReport

Report generated on 2017-03-27 07:12:26 using [dpcR](#) R package.

Detected input file: 20130918\_Dilution\_log10.csv.

md5 checksum of the input file: 6bf3306199dd7af439d1c8acd08e23c1

**The input was modified manually in dpcReport application.**

File format: QX100.

## Data summary table

Run	Experiment name	Replicate ID	Assay	Method	$\lambda$	$\lambda$ (lower CI)	$\lambda$ (upper CI)	Concentration	Concentration (lower CI)	Concentration (upper CI)	k	n
ABS1.A09.gDNA + P 10^4	ABS1	A09.gDNA + P 10^4	ileS	dube	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.A09.gDNA + P 10^4	ABS1	A09.gDNA + P 10^4	ileS	bhat	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.B09.gDNA	ABS1	B09.gDNA	ileS	bhat	0.07	0.07	0.08	1171.87	0.11	0.12	1110	11000

# Input file checksum

## Table of Contents

- [dpcReport](#)
  - [Data summary table](#)
    - [Explanation](#)
  - [Data summary scatter charts](#)
    - [Scatter chart](#)
  - [Compare runs](#)
  - [Compare digital PCR experiments](#)
    - [The mean number of template molecules per partition](#)
- [R code](#)
- [R Session](#)

## dpcReport

Report generated on 2017-03-27 07:12:26 using [dpcR](#) R package.

Detected input file: 20130918\_Dilution\_log10.csv.

md5 checksum of the input file: 6bf3306199dd7af439d1c8acd08e23c1

**The input was modified manually in dpcReport application.**

File format: QX100.

## Data summary table

Run	Experiment name	Replicate ID	Assay	Method	$\lambda$	$\lambda$ (lower CI)	$\lambda$ (upper CI)	Concentration	Concentration (lower CI)	Concentration (upper CI)	k	n
ABS1.A09.gDNA + P 10 <sup>4</sup>	ABS1	A09.gDNA + P 10 <sup>4</sup>	ileS	dube	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.A09.gDNA + P 10 <sup>4</sup>	ABS1	A09.gDNA + P 10 <sup>4</sup>	ileS	bhat	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.B09.gDNA	ABS1	B09.gDNA	ileS	bhat	0.07	0.07	0.08	1171.07	0.08	0.09	1110	11000

Changes in case of the manual alteration of the input file.

# Manual alterations inside dpcReport

## Table of Contents

- [dpcReport](#)
  - [Data summary table](#)
    - [Explanation](#)
  - [Data summary scatter charts](#)
    - [Scatter chart](#)
  - [Compare runs](#)
  - [Compare digital PCR experiments](#)
    - [The mean number of template molecules per partition](#)
- [R code](#)
- [R Session](#)

## dpcReport

Report generated on 2017-03-27 07:12:26 using [dpcR](#) R package.

Detected input file: 20130918\_Dilution\_log10.csv.

md5 checksum of the input file: 6bf3306199dd7af439d1c8acd08e23c1

**The input was modified manually in dpcReport application.**

File format: QX100.

## Data summary table

Run	Experiment name	Replicate ID	Assay	Method	$\lambda$	$\lambda$ (lower CI)	$\lambda$ (upper CI)	Concentration	Concentration (lower CI)	Concentration (upper CI)	k	n
ABS1.A09.gDNA + P 10 <sup>4</sup>	ABS1	A09.gDNA + P 10 <sup>4</sup>	ileS	dube	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.A09.gDNA + P 10 <sup>4</sup>	ABS1	A09.gDNA + P 10 <sup>4</sup>	ileS	bhat	0.07	0.07	0.08	970.44	0.08	0.09	936	13346
ABS1.B09.gDNA	ABS1	B09.gDNA	ileS	bhat	0.07	0.07	0.08	1171.87	0.11	0.12	1143	11888

## R Session

```
## R version 3.3.3 (2017-03-06)
## Platform: x86_64-pc-linux-gnu (64-bit)
## Running under: Ubuntu 14.04.5 LTS
##
## locale:
## [1] LC_CTYPE=pl_PL.UTF-8      LC_NUMERIC=C
## [3] LC_TIME=pl_PL.UTF-8      LC_COLLATE=pl_PL.UTF-8
## [5] LC_MONETARY=pl_PL.UTF-8  LC_MESSAGES=pl_PL.UTF-8
## [7] LC_PAPER=pl_PL.UTF-8     LC_NAME=C
## [9] LC_ADDRESS=C             LC_TELEPHONE=C
## [11] LC_MEASUREMENT=pl_PL.UTF-8 LC_IDENTIFICATION=C
##
## attached base packages:
## [1] stats      graphics  grDevices  utils      datasets  methods   base
##
## other attached packages:
## [1] xtable_1.8-2      knitr_1.15.1      digest_0.6.12
## [4] dplyr_0.5.0       DT_0.2            ggplot2_2.2.1
## [7] rhandsontable_0.3.4 shinythemes_1.1.1 shiny_1.0.0
## [10] dpcR_0.4
##
## loaded via a namespace (and not attached):
## [1] jsonlite_1.2      binom_1.1-1      splines_3.3.3
## [4] assertthat_0.1    highr_0.6        Rfit_0.23.0
## [7] chipPCR_0.0.8-11  yaml_2.1.14      outliers_0.14
## [10] robustbase_0.92-7 lattice_0.20-34  quantreg_5.29
## [13] quadprog_1.5-5    polyclip_1.5-6   colorspace_1.3-1
## [16] sandwich_2.3-4    htmltools_0.3.5  httpuv_1.3.3
## [19] Matrix_1.2-8      plyr_1.8.4       SparseM_1.74
## [22] mvtnorm_1.0-5     ptw_1.9-11       scales_0.4.1
## [25] tensor_1.5        pracma_1.9.5     MatrixModels_0.4-1
## [28] tibble_1.2        mgcv_1.8-16      TH.data_1.0-7
## [31] dgof_1.2          lazyeval_0.2.0   survival_2.40-1
## [34] magrittr_1.5      readxl_0.1.1     mime_0.5
## [37] deldir_0.1-12     evaluate_0.10    nlme_3.1-131
```

## Reproducibility of the workflow

An analysis conducted in a GUI-based software, as *dpcReport*, is more challenging to reproduce.

*dpcReport* exports all steps of the analysis, including parameters adjusted manually by the user, in form of the **R** code that recreates the whole workflow.

# Reproducibility of the workflow

## R code

The R code below may be used to recreate reported results.

```
# Load packages
library(dpcR)
# if you do not have dpcR package, install it from GitHub:
# devtools::install_github("michbur/dpcR")
library(ggplot2) # ggplot2 library for nice plots
# Define theme for plots
cool_theme <- theme(plot.background=element_rect(fill = "transparent", colour = "transparent"),
panel.grid.major = element_line(colour="lightgrey", linetype = "dashed"), panel.background =
element_rect(fill = "white", colour = "black"), legend.background = element_rect(fill="NA"),
legend.position = "bottom", axis.text = element_text(size = 14), axis.title.x = element_text(size=17,
vjust = -0.1), axis.title.y = element_text(size = 17, vjust = 1), strip.text = element_text(size = 17,
face = "bold"), strip.background = element_rect(fill = "#9ecae1", colour = "black"), legend.text =
element_text(size=14), legend.title = element_text(size = 17), plot.title = element_text(size = 22),
legend.key = element_rect(fill = "white", colour = "black", linetype = "dashed", size = 0.5))
# Read and adjust data
# The input file is assumed to be in the current R working directory
input_data <- read_dpcr("20130918_Dilution_log10.csv", format = "QX100")

#####
# Print only table from summary.dpcr function
summary(input_data, print = FALSE)[["summary"]]

#####
# Prepare data for plots
plot_data <- summary(input_data, print = FALSE)[["summary"]]
plot_data <- plot_data[plot_data[["method"]] == "dube", ]
ggplot(plot_data, aes(x = experiment, y = lambda, ymax = lambda.up, ymin = lambda.low)) + geom_point(size
= 4, alpha = 0.6, shape = 2, colour = "blue") + cool_theme + geom_boxplot(outlier.colour = NA, fill =
adjustcolor("lightgrey", alpha.f = 0.25), shape = 15) + ggtitle(paste0("Experiment boxplot\nCI method: ",
```

*dpcReport* is the integrated environment for the analysis of dPCR data.

Web server: [www.smorfland.uni.wroc.pl/shiny/dpcReport](http://www.smorfland.uni.wroc.pl/shiny/dpcReport)

R package (including your local instance of dpcReport):

[www.github.com/michbur/dpcR](https://www.github.com/michbur/dpcR)



## Acknowledgements and funding

This research was partially funded by the KNOW Consortium and National Science Center (2015/17/N/NZ2/01845).

- Małgorzata Kotulska.
- Paweł Mackiewicz,
- Stefan Rödiger,
- **biogram** package  
(<https://cran.r-project.org/package=biogram>):
  - Piotr Sobczyk,
  - Chris Lauber,
- **AmyLoad** database ([comprec-lin.iia.pwr.edu.pl/amyload](http://comprec-lin.iia.pwr.edu.pl/amyload)):
  - Paweł Woźniak,

### References

---

Família, C., Dennison, S. R., Quintas, A., and Phoenix, D. A. (2015). Prediction of Peptide and Protein Propensity for Amyloid Formation. *PLOS ONE*, 10(8):e0134679.

Garbuzynskiy, S. O., Lobanov, M. Y., and Galzitskaya, O. V. (2010). FoldAmyloid: a method of prediction of amyloidogenic regions from protein sequence. *Bioinformatics (Oxford, England)*, 26(3):326–332.

## References II

- Kosiol, C., Goldman, N., and Buttimore, N. H. (2004). A new criterion and method for amino acid classification. *Journal of Theoretical Biology*, 228(1):97–106.
- Melo, F. and Marti-Renom, M. A. (2006). Accuracy of sequence alignment and fold assessment using reduced amino acid alphabets. *Proteins*, 63(4):986–995.
- Paz, M. L. d. I. and Serrano, L. (2004). Sequence determinants of amyloid fibril formation. *Proceedings of the National Academy of Sciences*, 101(1):87–92.

## References III

- Sawaya, M. R., Sambashivan, S., Nelson, R., Ivanova, M. I., Sievers, S. A., Apostol, M. I., Thompson, M. J., Balbirnie, M., Wiltzius, J. J. W., McFarlane, H. T., Madsen, A. , Riek, C., and Eisenberg, D. (2007). Atomic structures of amyloid cross-spines reveal varied steric zippers. *Nature*, 447(7143):453–457.
- Stephenson, J. D. and Freeland, S. J. (2013). Unearthing the root of amino acid similarity. *Journal of Molecular Evolution*, 77(4):159–169.
- Walsh, I., Seno, F., Tosatto, S. C. E., and Trovato, A. (2014). PASTA 2.0: an improved server for protein aggregation prediction. *Nucleic Acids Research*, page gku399.