Supplement to: Algorithms for Automatized Detection of Hook Effect-bearing Amplification Curves

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Contents

1 Introduction

This is a supplement document for the study *Algorithms for Automatized Detection of Hook Effect-bearing Amplification Curves*. The functions and data presented in the paper are available from https://github.com/devSJR/PCRedux. The data, including the RDML file are part of the `PCRedux` package and are made available in the CSV or RDML format (Rödiger et al. 2017) for a vendor independent analysis.

All analysis were implemented and done with the **R** statistical computing language (R Core Team 2017, Rödiger et al. (2015)) and dedicated integrated development environments such as **RKWard** (Rödiger et al. 2012). Further documentation can be found in the help files of the **R** packages.

We added the source code for the generation of the figures in the main text at the end of the document.

> Note: Some rows in the tables below appear to be empty. This expected behaviour may occur in cases where the corresponding functions were not able to calculate the coefficients due to a failed model fit or violation of truncation criterion.

1.1 Results for the analysis of the hookreg.rdml data set by human rater

All calculations in the following sections were done with `hookreg.rdml` data set, which is part of the `PCRedux` package. The data were transfered to the **R** environment by the `RDML` package (Rödiger et al. 2017).

```
# Load the RDML package for reading of the hookreg.rdml-file from the PCRedux
# package. The magrittr package is used for pipes.

library(RDML)
library(PCRedux)
library(magrittr)
```

```
# A comprehensive description of the RDML-file import can be found in Rödiger
# et al. (2017) Bioinformatics

raw_data <- RDML$new(filename=system.file("hookreg.rdml", package="PCRedux"))

##
## Loading experiment: exp1
##   run: run1

raw_data_tab <- raw_data$AsTable(name.pattern=paste(
  react$position,
  react$sample$id,
  # run id added to names
  sep="~"))
data <- as.data.frame(raw_data$GetFData(raw_data_tab, long.table=FALSE))

# Plot all data of the hookreg.rdml-file
matplot(data[, 1], data[, -1], type="l", lty=1, lwd=2, ylab="RFU", xlab="Cycle")
```
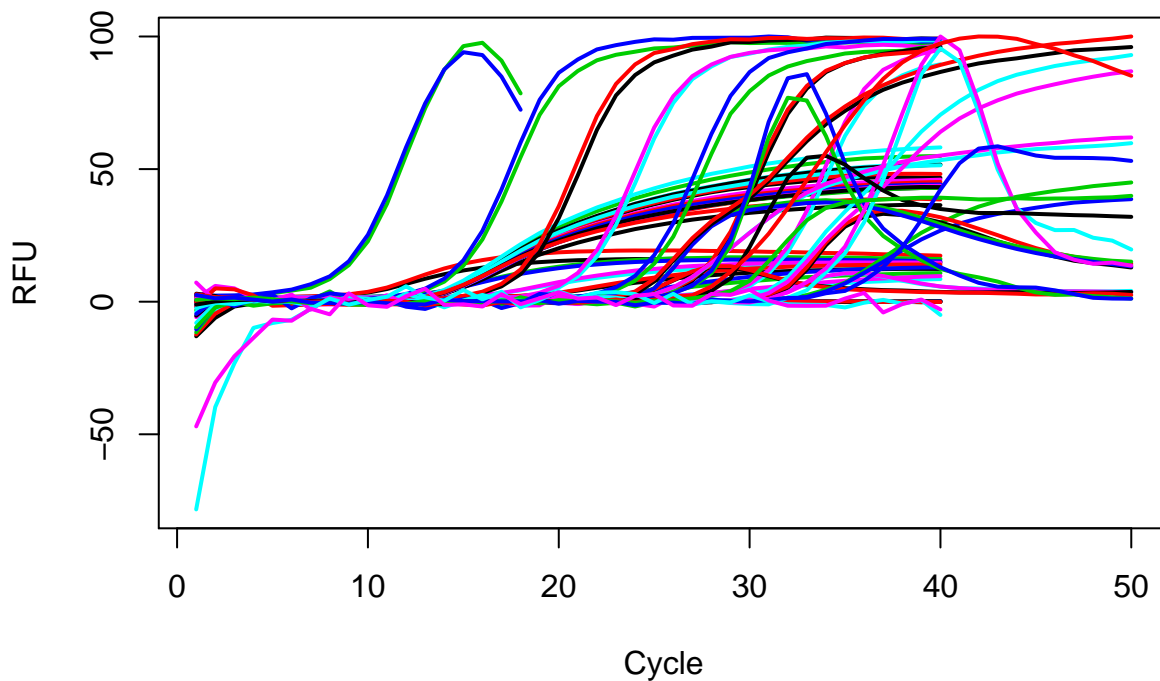

Give the first three and last three entires of the data for data evaluation

```
library(xtable)
options(xtable.comment=FALSE)
print(xtable(t(rbind(head(data, 10), tail(data, 10)))), scalebox='0.55', floating=FALSE)
```

	1	2	3	4	5	6	7	8	9	10	41	42	43	44	45	46	47	48	49	50
cyc	1.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	41.00	42.00	43.00	44.00	45.00	46.00	47.00	48.00	49.00	50.00
A01˜F1.1	1.70	1.69	1.69	1.69	1.72	1.78	1.89	2.14	2.59	3.42										
A02˜F1.2	1.74	1.74	1.75	1.76	1.80	1.84	1.99	2.26	2.79	3.72										
A03˜F2.1	1.72	1.69	1.69	1.69	1.69	1.67	1.70	1.72	1.77	1.87										
A04˜F2.2	1.66	1.65	1.65	1.62	1.64	1.63	1.65	1.66	1.72	1.80										
A05˜F3.1	1.67	1.69	1.67	1.65	1.64	1.65	1.64	1.65	1.63	1.64										
A06˜F3.2	1.68	1.67	1.66	1.65	1.64	1.65	1.65	1.62	1.63	1.65										
A07˜F4.1	1.72	1.71	1.68	1.69	1.69	1.67	1.67	1.67	1.68	1.68										
A08˜F4.2	1.71	1.71	1.68	1.68	1.67	1.68	1.67	1.66	1.67	1.66										
A09˜F5.1	1.69	1.69	1.69	1.66	1.66	1.66	1.67	1.66	1.65	1.65										
A10˜F5.2	1.73	1.73	1.70	1.68	1.68	1.69	1.68	1.66	1.68	1.68										
A11˜F6.1	1.72	1.68	1.66	1.66	1.66	1.66	1.64	1.65	1.65	1.66										
A12˜F6.2	1.66	1.65	1.62	1.61	1.63	1.62	1.60	1.60	1.60	1.60										
B01˜HP1	0.24	0.13	0.00	0.02	-0.04	-0.12	-0.12	-0.09	-0.06	-0.04										
B02˜HP2	0.29	0.25	0.01	-0.00	-0.08	-0.17	-0.19	-0.22	-0.12	-0.09										
B03˜HP3	0.25	0.24	0.04	-0.02	-0.09	-0.18	-0.23	-0.28	-0.23	-0.20										
B04˜HP4	0.28	0.21	0.02	0.00	-0.08	-0.15	-0.23	-0.23	-0.21	-0.17										
B05˜HP5	0.18	0.20	0.03	-0.01	-0.04	-0.17	-0.21	-0.21	-0.18	-0.14										
B06˜HP6	0.15	0.15	0.01	-0.01	-0.06	-0.09	-0.16	-0.14	-0.14	-0.11										
B07˜HP7	0.35	0.31	0.10	-0.04	-0.12	-0.24	-0.29	-0.32	-0.35	-0.33										
B08˜HP8	0.09	0.13	-0.01	-0.01	-0.06	-0.06	-0.12	-0.15	-0.10	-0.08										
B09˜HP9	0.10	0.14	0.01	-0.04	-0.04	-0.06	-0.14	-0.14	-0.06	-0.06										
B10˜HP10	0.24	0.23	0.02	-0.03	-0.06	-0.16	-0.27	-0.29	-0.27	-0.21										
B11˜HP11	-0.00	0.17	0.06	-0.00	-0.07	-0.16	-0.25	-0.29	-0.28	-0.22										
B12˜HP12	0.08	0.15	0.04	-0.00	-0.07	-0.12	-0.13	-0.19	-0.13	-0.08										
C01˜HP13	0.13	0.22	0.02	-0.01	-0.10	-0.14	-0.21	-0.23	-0.21	-0.14										
C02˜HP14	0.26	0.27	0.11	0.03	-0.18	-0.24	-0.32	-0.44	-0.38	-0.38										
C03˜HP15	0.19	0.16	0.01	-0.02	-0.07	-0.08	-0.11	-0.16	-0.15	-0.08										
C04˜HP16	0.03	0.16	0.03	-0.01	-0.04	-0.14	-0.23	-0.30	-0.26	-0.22										
C05˜HP17	0.19	0.21	0.03	-0.02	-0.08	-0.14	-0.14	-0.26	-0.25	-0.17										
C06˜HP18	-0.07	0.14	0.01	-0.00	-0.04	-0.11	-0.15	-0.24	-0.24	-0.16										
C07˜HP19	0.04	0.11	0.04	0.03	-0.04	-0.14	-0.14	-0.19	-0.12	-0.08										
C08˜HP20	-0.04	0.10	0.02	-0.03	-0.03	-0.06	-0.08	-0.10	-0.04	0.02										
C09˜HP21	0.23	0.24	0.04	-0.03	-0.10	-0.15	-0.18	-0.26	-0.22	-0.11										
C10˜HP22	-0.04	0.13	-0.01	-0.00	-0.05	-0.07	-0.12	-0.20	-0.18	-0.09										
C11˜HP23	0.44	0.31	0.01	0.03	-0.18	-0.16	-0.20	-0.27	-0.15	-0.02										
C12˜HP24	0.07	0.17	0.01	0.01	-0.10	-0.09	-0.16	-0.20	-0.20	-0.05										
D01˜HP25	-0.01	0.08	-0.03	-0.01	0.01	-0.05	-0.03	-0.09	-0.07	0.09										
D02˜HP26	0.08	0.17	0.03	-0.01	-0.07	-0.12	-0.12	-0.18	-0.20	-0.05										
D03˜HP27	0.12	0.16	0.01	-0.01	-0.06	-0.10	-0.09	-0.13	-0.02	0.07										
D04˜HP28	0.17	0.21	0.03	0.01	-0.09	-0.16	-0.17	-0.25	-0.22	-0.10										
D05˜HP29	0.29	0.20	0.04	-0.02	-0.06	-0.16	-0.20	-0.30	-0.24	-0.16										
D06˜HP30	0.42	0.24	0.03	-0.01	-0.09	-0.16	-0.24	-0.22	-0.22	-0.14										
D07˜HP31	0.21	0.18	0.04	-0.02	-0.07	-0.13	-0.16	-0.20	-0.18	-0.09										
D08˜HP32	0.25	0.11	-0.01	-0.00	-0.05	-0.08	-0.08	-0.08	0.03	0.11										
D09˜F1.1_td	-0.51	-0.32	-0.13	-0.01	0.19	0.27	0.43	0.52	0.71	1.01										
D10˜F1.2_td	-0.49	-0.30	-0.16	-0.03	0.19	0.30	0.45	0.59	0.77	1.12										
D11˜F1.3_td	-0.04	0.13	0.11	-0.02	-0.11	-0.11	-0.09	0.09	0.04	-0.19										
D12˜F1.4_td	0.06	0.03	0.25	0.01	0.08	-0.01	0.01	-0.05	0.00	-0.04										
E01˜F2.1_td	-0.23	-0.16	-0.08	-0.01	0.12	0.13	0.22	0.24	0.32	0.38										
E02˜F2.2_td	-0.24	-0.15	-0.07	-0.03	0.10	0.14	0.20	0.26	0.31	0.38										
E03˜F2.3_td	-0.06	-0.04	0.12	0.04	0.12	-0.09	-0.13	-0.01	-0.08	-0.02										
E04˜F2.4_td	0.04	0.05	-0.03	-0.12	0.15	0.13	-0.06	-0.14	-0.01	-0.06										
E05˜F3.1_td	-0.18	-0.13	-0.08	-0.00	0.09	0.11	0.19	0.21	0.25	0.30										
E06˜F3.2_td	-0.20	-0.12	-0.06	-0.02	0.09	0.11	0.16	0.19	0.22	0.26										
E07˜F3.3_td	0.01	-0.13	0.01	0.09	-0.03	-0.12	0.07	0.01	0.00	-0.10										
E08˜F3.4_td	-0.07	0.01	0.12	-0.00	0.10	-0.04	0.03	-0.06	0.04	0.08										
E09˜F4.1_td	-0.18	-0.10	-0.06	-0.00	0.08	0.09	0.17	0.19	0.24	0.25										
E10˜F4.2_td	-0.21	-0.13	-0.06	-0.03	0.09	0.12	0.18	0.21	0.25	0.30										
E11˜F4.3_td	0.06	0.06	0.08	-0.10	-0.06	-0.09	0.00	-0.04	0.14	0.19										
E12˜F4.4_td	-0.05	-0.04	0.05	0.03	0.04	0.11	-0.12	0.03	0.09	-0.06										
F01˜F5.1_td	-0.18	-0.14	-0.06	-0.01	0.09	0.11	0.17	0.20	0.24	0.26										
F02˜F5.2_td	-0.20	-0.12	-0.06	-0.03	0.08	0.13	0.17	0.20	0.22	0.26										
F03˜F5.3_td	-0.09	-0.03	-0.01	-0.06	-0.04	0.03	0.09	-0.00	0.06	0.05										
F04˜F5.4_td	-0.08	-0.03	-0.07	0.11	-0.09	-0.03	-0.09	-0.08	0.07	0.03										
F05˜F6.1_td	-0.18	-0.12	-0.05	-0.02	0.08	0.12	0.18	0.18	0.23	0.27										
F06˜F6.2_td	-0.22	-0.13	-0.06	-0.01	0.08	0.12	0.19	0.22	0.25	0.29										
F07˜F6.3_td	0.03	-0.14	0.05	-0.04	-0.06	-0.06	0.09	0.03	0.05	0.05										
F08˜F6.4_td	-0.08	0.07	0.01	0.19	-0.02	-0.15	0.09	-0.07	-0.06	0.07										
F09˜WGA	2.07	2.04	2.17	2.53	3.23	4.18	5.27	8.52	13.81	22.77										
F10˜WGA	2.35	2.29	2.38	2.72	3.53	4.56	6.57	9.56	15.25	25.23										
F11˜1ng/mkl	-9.69	-3.48	-0.93	-0.28	0.04	0.32	0.03	0.12	0.19	0.12	5.17	4.97	4.68	4.56	4.26	4.07	3.93	3.80	3.90	4.07
F12˜1ng/mkl	-5.83	-1.24	-0.58	0.36	-0.18	-0.12	-0.08	0.30	-0.28	0.00	5.13	4.69	4.46	4.00	3.97	3.90	3.91	3.85	3.72	3.64
G01˜100 ng/mkl	-5.30	0.73	0.38	0.37	-0.25	-0.05	-0.39	-0.35	0.33	0.07	3.52	3.47	3.55	3.58	3.41	3.32	3.24	3.38	3.47	3.67
G02˜100 ng/mkl	2.08	1.41	-0.05	0.11	-0.24	0.02	-0.28	0.22	0.32	0.09	3.40	3.38	3.19	3.01	2.73	2.73	2.92	3.19	2.99	2.51
G03˜1ng/mkl	-3.15	0.13	0.25	0.77	0.63	-0.18	-0.20	-0.18	-0.01	-0.25	33.08	35.84	37.98	39.55	40.70	41.78	42.61	43.57	44.27	44.95
G04˜1ng/mkl	-1.47	1.06	0.33	0.34	-0.10	0.05	0.06	0.14	-0.09	-0.19	29.44	31.48	33.10	34.28	35.43	36.48	37.37	37.85	38.30	38.66
G05˜100 ng/mkl	-3.89	0.03	-0.06	-0.15	0.33	-0.00	0.09	0.21	-0.31	-0.08	54.33	55.24	56.27	56.94	57.54	57.95	58.26	58.65	59.11	59.78
G06˜100 ng/mkl	1.14	5.95	5.03	1.33	-0.93	-1.42	-0.96	-1.06	-0.99	-0.42	56.05	56.92	57.93	58.62	59.34	59.89	60.68	61.15	61.71	61.93
G07˜1ng/mkl	-13.06	-6.09	-1.82	-0.66	-0.45	-0.12	0.03	0.20	0.20	0.40	27.73	25.30	22.76	20.66	18.77	17.01	15.44	14.52	13.79	12.90
G08˜1ng/mkl	-12.37	-4.51	-0.46	-0.38	-0.58	-0.08	0.29	-0.11	-0.09	0.19	29.86	27.49	25.07	22.50	20.20	18.29	16.91	15.85	14.96	14.26
G09˜100 ng/mkl	-11.54	-2.08	0.48	0.73	0.15	-0.31	-0.14	-0.02	0.27	-0.09	26.88	24.58	22.69	20.93	19.49	18.21	16.99	16.14	15.44	15.08
G10˜100 ng/mkl	-10.43	-1.72	0.77	-0.08	-0.02	-0.27	-0.11	0.35	0.04	0.32	25.75	23.63	21.66	19.89	18.35	17.04	16.09	15.04	14.20	13.33
G11˜1ng/mkl	-8.02	-0.61	0.12	0.04	-0.75	-0.05	-0.01	-0.02	0.37	-0.19	75.63	79.88	83.18	85.59	87.26	88.88	90.08	91.05	91.92	93.02
G12˜1ng/mkl	-1.57	1.20	0.30	0.43	0.18	0.17	-0.13	0.25	0.21	-0.16	69.08	72.91	75.94	78.47	80.38	81.99	83.52	84.84	86.00	86.88
H01˜100 ng/mkl	3.01	2.14	-0.30	0.40	0.38	-0.39	-0.14	0.35	0.22	-0.04	88.33	89.85	90.92	91.77	92.80	93.77	94.77	95.14	95.57	96.02
H02˜100 ng/mkl	-1.97	5.01	4.66	2.37	-1.53	-1.31	-1.11	-0.85	-1.18	-1.00	91.09	92.77	94.18	95.33	96.21	97.21	97.79	98.54	99.17	100.00
H03˜s1	-9.68	-2.16	-0.04	-1.52	-0.61	-0.26	0.64	3.88	-0.26	0.29	10.47	9.17	7.58	5.40	3.52	2.60	2.68	2.10	1.64	1.23
H04˜s2	-4.61	0.75	-1.59	0.78	2.69	-2.51	1.27	3.16	2.36	0.05	9.87	7.11	5.65	5.42	5.32	4.27	2.89	1.47	1.19	1.12
H05˜s3	-2.40	-0.32	-0.94	0.37	-0.12	-0.13	-1.57	0.27	1.64	1.11	90.47	71.57	49.81	35.28	29.68	26.99	27.04	24.12	23.04	19.67
H06˜s4	7.22	0.26	0.86	1.10	0.56	2.69	-3.01	1.52	0.55	-0.15	94.82	75.19	52.09	35.02	26.07	18.63	15.83	14.30	14.73	13.59
H07˜s5	-1.10	0.11	0.59	0.78	0.04	0.21	0.24	-0.03	-0.49	0.47	34.14	33.45	33.43	33.39	33.10	32.88	32.64	32.49	32.22	32.00
H08˜s6	2.78	1.73	1.47	0.77	0.49	0.52	-0.01	0.11	-0.56	-0.61	99.20	100.00	99.93	99.12	97.15	95.36	92.91	90.75	87.92	85.20
H09˜s7	0.70	1.27	0.96	1.55	0.95	0.15	-0.57	-0.25	-1.05	-1.25	38.91	38.57	38.63	39.02	38.77	38.91	38.94	39.18	39.37	39.91
H10˜s8	2.51	1.27	1.53	0.79	0.08	0.83	-0.33	-0.54	-0.72	-0.02	52.22	57.73	58.59	56.83	55.11	54.27	54.25	54.15	53.90	53.08
H11˜NTC	-78.32	-39.71	-23.30	-9.87	-8.05	-6.83	-2.73	1.25	-1.12	0.62										
H12˜NTC	-47.02	-30.47	-20.59	-13.65	-6.74	-7.18	-2.64	-4.76	3.15	-1.36										

Printout of all measured samples, their rating by two humans (rater 1 and rater 2) with their dichotomous ratings (0, no hook; 1, hook) and their sources.

- The boggy data (qpcR::boggy) set was taken from the `qpcR` package (Ritz and Spiess 2008, Spiess, Feig, and Ritz (2008)).
- The C127EGHP data (chipPCR::C127EGHP) set was taken from the `chipPCR` package (Rödiger, Burdukiewicz, and Schierack 2015).
- The testdat data (qpcR::testdat) set was taken from the `qpcR` package (Ritz and Spiess 2008, Spiess, Feig, and Ritz (2008)).
- Other data were prepared by Evrogen laboratory experiments.

#	Sample	Data Source	Target	Chemistry	Hook effect-like Rater 1	Hook effect-like Rater 2	Rating Conformity
1	F1.1	qpcR::boggy	synthetic template	Syto-13	1	1	1
2	F1.2	qpcR::boggy	synthetic template	Syto-13	1	1	1
3	F2.1	qpcR::boggy	synthetic template	Syto-13	1	1	1
4	F2.2	qpcR::boggy	synthetic template	Syto-13	1	1	1
5	F3.1	qpcR::boggy	synthetic template	Syto-13	0	0	1
6	F3.2	qpcR::boggy	synthetic template	Syto-13	0	0	1
7	F4.1	qpcR::boggy	synthetic template	Syto-13	0	0	1
8	F4.2	qpcR::boggy	synthetic template	Syto-13	0	0	1
9	F5.1	qpcR::boggy	synthetic template	Syto-13	0	0	1
10	F5.2	qpcR::boggy	synthetic template	Syto-13	0	0	1
11	F6.1	qpcR::boggy	synthetic template	Syto-13	0	0	1
12	F6.2	qpcR::boggy	synthetic template	Syto-13	0	0	1
13	HP1	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
14	HP2	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
15	HP3	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
16	HP4	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
17	HP5	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
18	HP6	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
19	HP7	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
20	HP8	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
21	HP9	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
22	HP10	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
23	HP11	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
24	HP12	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
25	HP13	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
26	HP14	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
27	HP15	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
28	HP16	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
29	HP17	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
30	HP18	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
31	HP19	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
32	HP20	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
33	HP21	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
34	HP22	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
35	HP23	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
36	HP24	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
37	HP25	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
38	HP26	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
39	HP27	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
40	HP28	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
41	HP29	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
42	HP30	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
43	HP31	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
44	HP32	chipPCR::C127EGHP	MLC-2v	TaqMan (Cy5/BHQ2)	0	0	1
45	F1.1_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
46	F1.2_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
47	F1.3_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
48	F1.4_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
49	F2.1_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
50	F2.2_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
51	F2.3_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
52	F2.4_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
53	F3.1_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
54	F3.2_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
55	F3.3_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
56	F3.4_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
57	F4.1_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
58	F4.2_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
59	F4.3_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
60	F4.4_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
61	F5.1_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
62	F5.2_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
63	F5.3_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
64	F5.4_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
65	F6.1_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
66	F6.2_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
67	F6.3_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
68	F6.4_td	qpcR::testdat	S27a housekeeping gene	SybrGreen I	0	0	1
69	F09~WGA	Evrogen lab experiment	Whole genome amplification	EvaGreen	1	1	1
70	F10~WGA	Evrogen lab experiment	Whole genome amplification	EvaGreen	1	1	1
71	F11~1ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	1	1	1
72	F12~1ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	1	1	1
73	G01~100ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	1	1	1
74	G02~100ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	1	1	1
75	G03~1ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	0	0	1
76	G04~1ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	0	0	1
77	G05~100ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	0	0	1
78	G06~100ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	0	0	1
79	G07~1ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	1	1	1
80	G08~1ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	1	1	1
81	G09~100ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	1	1	1
82	G10~100ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	1	1	1
83	G11~1ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	0	0	1
84	G12~1ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	0	0	1
85	H01~100ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	0	0	1
86	H02~100ng/mkl	Evrogen lab experiment	BRCA1 gene	TaqMan (HEX/BHQ1)	0	0	1
87	s1	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	1	1	1
88	s2	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	1	1	1
89	s3	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	1	1	1
90	s4	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	1	1	1
91	s5	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	1	1	1
92	s6	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	1	1	1
93	s7	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	0	0	1
94	s8	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	1	1	1
95	NTC	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	0	0	1
96	NTC	Evrogen lab experiment	NRAS gene	TaqMan (FAM/BHQ1)	0	0	1

1.2 Results for the analysis of the hookreg.rdml data set with hookreg

```r
library(PCRedux)
library(magrittr)
suppressMessages(library(qpcR))

res_hookreg <- sapply(2L:ncol(data), function(i) {
  hookreg(x=data[, 1], y=data[, i])
}) %>% t %>% data.frame(sample=colnames(data)[-1],.)



res_hookreg_table <- data.frame(sample=as.character(res_hookreg[["sample"]]),
                                intercept=signif(res_hookreg[["intercept"]], 2),
                                slope=signif(res_hookreg[["slope"]], 1),
                                hook.start=signif(res_hookreg[["hook.start"]], 0),
                                hook.delta=signif(res_hookreg[["hook.delta"]], 0),
                                p.value=signif(res_hookreg[["p.value"]], 4),
                                CI.low=signif(res_hookreg[["CI.low"]], 2),
                                CI.up=signif(res_hookreg[["CI.up"]], 2),
                                hook.fit=res_hookreg[["hook.fit"]],
                                hook.CI=res_hookreg[["hook.CI"]],
                                hook=res_hookreg[["hook"]]
)
```

Printout of all measured samples and their sources.

```r
library(xtable)
options(xtable.comment=FALSE)
print(xtable(res_hookreg_table),
      size = "normalsize",
      include.rownames = FALSE,
      include.colnames = TRUE,
      caption.placement = "top",
      comment=FALSE,
      table.placement = "!ht", scalebox='0.55', floating=FALSE
)
```

sample	intercept	slope	hook.start	hook.delta	p.value	CI.low	CI.up	hook.fit	hook.CI	hook
A01˜F1.1	1.20	-0.01	30.00	20.00	0.00	1.20	-0.01	1.00	1.00	1.00
A02˜F1.2	1.20	-0.01	30.00	20.00	0.00	1.20	-0.01	1.00	1.00	1.00
A03˜F2.1	1.20	-0.01	30.00	9.00	0.00	1.20	-0.00	1.00	1.00	1.00
A04˜F2.2	1.20	-0.01	30.00	9.00	0.00	1.20	-0.00	1.00	1.00	1.00
A05˜F3.1	1.10	-0.00	40.00	6.00	0.05	1.20	0.00	0.00	0.00	0.00
A06˜F3.2	1.10	-0.00	40.00	6.00	0.02	1.20	0.00	0.00	0.00	0.00
A07˜F4.1								0.00	0.00	0.00
A08˜F4.2								0.00	0.00	0.00
A09˜F5.1								0.00	0.00	0.00
A10˜F5.2								0.00	0.00	0.00
A11˜F6.1								0.00	0.00	0.00
A12˜F6.2								0.00	0.00	0.00
B01˜HP1								0.00	0.00	0.00
B02˜HP2								0.00	0.00	0.00
B03˜HP3								0.00	0.00	0.00
B04˜HP4								0.00	0.00	0.00
B05˜HP5								0.00	0.00	0.00
B06˜HP6								0.00	0.00	0.00
B07˜HP7								0.00	0.00	0.00
B08˜HP8								0.00	0.00	0.00
B09˜HP9								0.00	0.00	0.00
B10˜HP10								0.00	0.00	0.00
B11˜HP11								0.00	0.00	0.00
B12˜HP12								0.00	0.00	0.00
C01˜HP13								0.00	0.00	0.00
C02˜HP14								0.00	0.00	0.00
C03˜HP15								0.00	0.00	0.00
C04˜HP16								0.00	0.00	0.00
C05˜HP17								0.00	0.00	0.00
C06˜HP18								0.00	0.00	0.00
C07˜HP19								0.00	0.00	0.00
C08˜HP20								0.00	0.00	0.00
C09˜HP21								0.00	0.00	0.00
C10˜HP22								0.00	0.00	0.00
C11˜HP23								0.00	0.00	0.00
C12˜HP24								0.00	0.00	0.00
D01˜HP25								0.00	0.00	0.00
D02˜HP26								0.00	0.00	0.00
D03˜HP27								0.00	0.00	0.00
D04˜HP28								0.00	0.00	0.00
D05˜HP29								0.00	0.00	0.00
D06˜HP30								0.00	0.00	0.00
D07˜HP31								0.00	0.00	0.00
D08˜HP32								0.00	0.00	0.00
D09˜F1.1_td	1.00	-0.00	30.00	7.00	0.01	1.10	0.00	0.00	0.00	0.00
D10˜F1.2_td	1.10	-0.00	30.00	10.00	0.00	1.10	-0.00	1.00	1.00	1.00
D11˜F1.3_td	0.73	-0.02	10.00	30.00	0.05	1.50	0.01	0.00	0.00	0.00
D12˜F1.4_td	0.08	-0.00	3.00	40.00	0.42	0.40	0.01	0.00	0.00	0.00
E01˜F2.1_td	1.00	-0.00	30.00	7.00	0.04	1.10	0.00	0.00	0.00	0.00
E02˜F2.2_td	1.10	-0.00	40.00	5.00	0.15	1.30	0.00	0.00	0.00	0.00
E03˜F2.3_td	-0.13	0.00	20.00	20.00	0.90	1.40	0.06	0.00	0.00	0.00
E04˜F2.4_td	3.10	-0.08	30.00	8.00	0.24	12.00	0.17	0.00	0.00	0.00
E05˜F3.1_td								0.00	0.00	0.00
E06˜F3.2_td								0.00	0.00	0.00
E07˜F3.3_td	0.55	-0.02	10.00	30.00	0.09	1.40	0.01	0.00	0.00	0.00
E08˜F3.4_td	0.11	-0.00	10.00	30.00	0.84	1.00	0.03	0.00	0.00	0.00
E09˜F4.1_td								0.00	0.00	0.00
E10˜F4.2_td								0.00	0.00	0.00
E11˜F4.3_td	2.90	-0.08	30.00	10.00	0.14	9.50	0.11	0.00	0.00	0.00
E12˜F4.4_td	0.26	-0.02	6.00	40.00	0.08	1.20	0.01	0.00	0.00	0.00
F01˜F5.1_td								0.00	0.00	0.00
F02˜F5.2_td								0.00	0.00	0.00
F03˜F5.3_td	2.20	-0.06	30.00	10.00	0.06	5.60	0.04	0.00	0.00	0.00
F04˜F5.4_td	-0.08	0.00	20.00	20.00	0.89	1.50	0.06	0.00	0.00	0.00
F05˜F6.1_td								0.00	0.00	0.00
F06˜F6.2_td								0.00	0.00	0.00
F07˜F6.3_td	0.67	-0.02	20.00	20.00	0.24	2.20	0.03	0.00	0.00	0.00
F08˜F6.4_td	0.09	-0.00	4.00	40.00	0.73	0.62	0.02	0.00	0.00	0.00
F09˜WGA								0.00	0.00	0.00
F10˜WGA								0.00	0.00	0.00
F11˜1ng/mkl	2.40	-0.04	40.00	20.00	0.00	3.20	-0.02	1.00	1.00	1.00
F12˜1ng/mkl	2.30	-0.04	40.00	20.00	0.00	3.30	-0.02	1.00	1.00	1.00
G01˜100 ng/mkl	1.60	-0.03	30.00	20.00	0.00	2.10	-0.02	1.00	1.00	1.00
G02˜100 ng/mkl	1.70	-0.03	30.00	20.00	0.00	2.20	-0.02	1.00	1.00	1.00
G03˜1ng/mkl								0.00	0.00	0.00
G04˜1ng/mkl								0.00	0.00	0.00
G05˜100 ng/mkl								0.00	0.00	0.00
G06˜100 ng/mkl								0.00	0.00	0.00
G07˜1ng/mkl	3.00	-0.05	40.00	10.00	0.00	3.30	-0.05	1.00	1.00	1.00
G08˜1ng/mkl	3.00	-0.05	40.00	10.00	0.00	3.30	-0.04	1.00	1.00	1.00
G09˜100 ng/mkl	2.50	-0.04	30.00	20.00	0.00	2.70	-0.04	1.00	1.00	1.00
G10˜100 ng/mkl	2.60	-0.05	30.00	20.00	0.00	2.80	-0.04	1.00	1.00	1.00
G11˜1ng/mkl								0.00	0.00	0.00
G12˜1ng/mkl								0.00	0.00	0.00
H01˜100 ng/mkl								0.00	0.00	0.00
H02˜100 ng/mkl								0.00	0.00	0.00
H03˜s1	2.40	-0.05	30.00	20.00	0.00	3.30	-0.03	1.00	1.00	1.00
H04˜s2	2.20	-0.05	30.00	20.00	0.00	3.20	-0.02	1.00	1.00	1.00
H05˜s3	4.10	-0.08	40.00	10.00	0.00	6.20	-0.04	1.00	1.00	1.00
H06˜s4	4.60	-0.09	40.00	10.00	0.00	6.80	-0.04	1.00	1.00	1.00
H07˜s5	1.60	-0.02	30.00	20.00	0.00	2.10	-0.01	1.00	1.00	1.00
H08˜s6	1.80	-0.02	40.00	9.00	0.00	2.10	-0.01	1.00	1.00	1.00
H09˜s7								0.00	0.00	0.00
H10˜s8	1.50	-0.01	40.00	8.00	0.00	1.90	-0.00	1.00	1.00	1.00
H11˜NTC	0.92	-0.03	10.00	30.00	0.00	1.50	-0.01	1.00	1.00	1.00
H12˜NTC	0.50	-0.01	10.00	30.00	0.19	1.50	0.02	0.00	0.00	0.00

1.3 Results for the analysis of the hookreg.rdml data set with hookregNL

```r
res_hookregNL <- suppressMessages(sapply(2L:ncol(data), function(i) {
  hookregNL(x=data[, 1], y=data[, i])
}) %>% t %>% data.frame(sample=colnames(data)[-1],.))

res_hookregNL_table <- data.frame(sample=as.character(res_hookregNL[["sample"]]),
                                  slope=signif(as.numeric(res_hookregNL[["slope"]]), 1),
                                  CI.low=signif(as.numeric(res_hookregNL[["CI.low"]]), 2),
                                  CI.up=signif(as.numeric(res_hookregNL[["CI.up"]]), 2),
                                  hook.CI=unlist(res_hookregNL[["hook"]])
)
```

```r
library(xtable)
options(xtable.comment=FALSE)

print(xtable(res_hookregNL_table),
      size = "normalsize",
      include.rownames = FALSE,
      include.colnames = TRUE,
      caption.placement = "top",
      comment=FALSE,
      table.placement = "!ht", scalebox='0.55', floating=FALSE
)
```

sample	slope	CI.low	CI.up	hook.CI
A01~F1.1	-0.10	-0.16	-0.12	1.00
A02~F1.2	-0.20	-0.19	-0.15	1.00
A03~F2.1	-0.09	-0.13	-0.06	1.00
A04~F2.2	-0.09	-0.12	-0.06	1.00
A05~F3.1	-0.02	-0.05	0.00	0.00
A06~F3.2	-0.02	-0.05	0.01	0.00
A07~F4.1	0.00			0.00
A08~F4.2	0.00	-0.01	0.02	0.00
A09~F5.1	0.01			0.00
A10~F5.2	0.01			0.00
A11~F6.1	0.00			0.00
A12~F6.2	0.00			0.00
B01~HP1	0.01			0.00
B02~HP2	0.08			0.00
B03~HP3	0.06			0.00
B04~HP4	0.03			0.00
B05~HP5	0.04			0.00
B06~HP6	0.02			0.00
B07~HP7	-0.10			0.00
B08~HP8	0.03			0.00
B09~HP9	0.05			0.00
B10~HP10	0.05			0.00
B11~HP11	0.06			0.00
B12~HP12	0.07			0.00
C01~HP13	0.05			0.00
C02~HP14	-0.04			0.00
C03~HP15	0.08			0.00
C04~HP16	0.09			0.00
C05~HP17	0.05			0.00
C06~HP18	0.03			0.00
C07~HP19	0.10			0.00
C08~HP20	0.02			0.00
C09~HP21	0.06			0.00
C10~HP22	0.01			0.00
C11~HP23	0.10			0.00
C12~HP24	0.06			0.00
D01~HP25	0.09			0.00
D02~HP26	0.10			0.00
D03~HP27	0.10			0.00
D04~HP28	0.10			0.00
D05~HP29	0.20			0.00
D06~HP30	0.10			0.00
D07~HP31	0.10			0.00
D08~HP32	0.04			0.00
D09~F1.1_td	0.09	0.02	0.16	0.00
D10~F1.2_td	-0.05			0.00
D11~F1.3_td				0.00
D12~F1.4_td				0.00
E01~F2.1_td	0.10	0.07	0.22	0.00
E02~F2.2_td	0.05			0.00
E03~F2.3_td	-0.00			0.00
E04~F2.4_td				0.00
E05~F3.1_td	0.10	0.07	0.21	0.00
E06~F3.2_td	0.09	0.05	0.14	0.00
E07~F3.3_td	-0.00			0.00
E08~F3.4_td	-0.00			0.00
E09~F4.1_td	0.10	0.03	0.16	0.00
E10~F4.2_td	0.08	0.03	0.13	0.00
E11~F4.3_td	-0.00			0.00
E12~F4.4_td	0.00			0.00
F01~F5.1_td	0.05	0.02	0.09	0.00
F02~F5.2_td	0.05			0.00
F03~F5.3_td	-0.01			0.00
F04~F5.4_td				0.00
F05~F6.1_td	0.03			0.00
F06~F6.2_td	0.03			0.00
F07~F6.3_td				0.00
F08~F6.4_td	-0.04			0.00
F09~WGA	-20.00	-38.00	-9.50	1.00
F10~WGA	-20.00	-32.00	-10.00	1.00
F11~1ng/mkl	-0.40			0.00
F12~1ng/mkl	-0.40			0.00
G01~100 ng/mkl	-0.40			0.00
G02~100 ng/mkl	-0.40			0.00
G03~1ng/mkl	0.02	-0.00	0.03	0.00
G04~1ng/mkl	-0.01			0.00
G05~100 ng/mkl	0.03			0.00
G06~100 ng/mkl	0.10			0.00
G07~1ng/mkl	-1.00			0.00
G08~1ng/mkl	-1.00			0.00
G09~100 ng/mkl	-1.00			0.00
G10~100 ng/mkl	-1.00			0.00
G11~1ng/mkl	-0.03			0.00
G12~1ng/mkl	-0.02			0.00
H01~100 ng/mkl	-0.10			0.00
H02~100 ng/mkl	0.01			0.00
H03~s1	-4.00			0.00
H04~s2	-4.00			0.00
H05~s3	-5.00			0.00
H06~s4	-8.00			0.00
H07~s5	-0.80			0.00
H08~s6	-0.50	-0.88	-0.13	1.00
H09~s7	0.05	0.01	0.08	0.00
H10~s8	-0.04			0.00
H11~NTC	40.00			0.00
H12~NTC	40.00			0.00

1.4 Comparison of the methods

```r
library(xtable)
options(xtable.comment=FALSE)

print(xtable(res, digits=0),
      size = "normalsize",
      include.rownames = FALSE,
      include.colnames = TRUE,
      caption.placement = "top",
      comment=FALSE,
      table.placement = "!ht", scalebox='0.55', floating=FALSE
)
```

Sample	Human rater	hookreg	hookregNL
F1.1	1	1	1
F1.2	1	1	1
F2.1	1	1	1
F2.2	1	1	1
F3.1	0	0	0
F3.2	0	0	0
F4.1	0	0	0
F4.2	0	0	0
F5.1	0	0	0
F5.2	0	0	0
F6.1	0	0	0
F6.2	0	0	0
HP1	0	0	0
HP2	0	0	0
HP3	0	0	0
HP4	0	0	0
HP5	0	0	0
HP6	0	0	0
HP7	0	0	0
HP8	0	0	0
HP9	0	0	0
HP10	0	0	0
HP11	0	0	0
HP12	0	0	0
HP13	0	0	0
HP14	0	0	0
HP15	0	0	0
HP16	0	0	0
HP17	0	0	0
HP18	0	0	0
HP19	0	0	0
HP20	0	0	0
HP21	0	0	0
HP22	0	0	0
HP23	0	0	0
HP24	0	0	0
HP25	0	0	0
HP26	0	0	0
HP27	0	0	0
HP28	0	0	0
HP29	0	0	0
HP30	0	0	0
HP31	0	0	0
HP32	0	0	0
F1.1_td	0	0	0
F1.2_td	0	1	0
F1.3_td	0	0	0
F1.4_td	0	0	0
F2.1_td	0	0	0
F2.2_td	0	0	0
F2.3_td	0	0	0
F2.4_td	0	0	0
F3.1_td	0	0	0
F3.2_td	0	0	0
F3.3_td	0	0	0
F3.4_td	0	0	0
F4.1_td	0	0	0
F4.2_td	0	0	0
F4.3_td	0	0	0
F4.4_td	0	0	0
F5.1_td	0	0	0
F5.2_td	0	0	0
F5.3_td	0	0	0
F5.4_td	0	0	0
F6.1_td	0	0	0
F6.2_td	0	0	0
F6.3_td	0	0	0
F6.4_td	0	0	0
F09˜WGA	1	0	1
F10˜WGA	1	0	1
F11˜1ng/mkl	1	1	0
F12˜1ng/mkl	1	1	0
G01˜100ng/mkl	1	1	0
G02˜100ng/mkl	1	1	0
G03˜1ng/mkl	0	0	0
G04˜1ng/mkl	0	0	0
G05˜100ng/mkl	0	0	0
G06˜100ng/mkl	0	0	0
G07˜1ng/mkl	1	1	0
G08˜1ng/mkl	1	1	0
G09˜100ng/mkl	1	1	0
G10˜100ng/mkl	1	1	0
G11˜1ng/mkl	0	0	0
G12˜1ng/mkl	0	0	0
H01˜100ng/mkl	0	0	0
H02˜100ng/mkl	0	0	0
s1	1	1	0
s2	1	1	0
s3	1	1	0
s4	1	1	0
s5	1	1	0
s6	1	1	1
s7	0	0	0
s8	1	1	0
NTC	0	1	0
NTC	0	0	0

```r
library(xtable)
options(xtable.comment=FALSE)

print(xtable(res_out, digits=0), scalebox='0.55', floating=FALSE)
```

	Sample	Human rater	hookreg	hookregNL	hookreg and hoohkreNL combined
1	F1.1	1	1	1	1
2	F1.2	1	1	1	1
3	F2.1	1	1	1	1
4	F2.2	1	1	1	1
5	F3.1	0	0	0	0
6	F3.2	0	0	0	0
7	F4.1	0	0	0	0
8	F4.2	0	0	0	0
9	F5.1	0	0	0	0
10	F5.2	0	0	0	0
11	F6.1	0	0	0	0
12	F6.2	0	0	0	0
13	HP1	0	0	0	0
14	HP2	0	0	0	0
15	HP3	0	0	0	0
16	HP4	0	0	0	0
17	HP5	0	0	0	0
18	HP6	0	0	0	0
19	HP7	0	0	0	0
20	HP8	0	0	0	0
21	HP9	0	0	0	0
22	HP10	0	0	0	0
23	HP11	0	0	0	0
24	HP12	0	0	0	0
25	HP13	0	0	0	0
26	HP14	0	0	0	0
27	HP15	0	0	0	0
28	HP16	0	0	0	0
29	HP17	0	0	0	0
30	HP18	0	0	0	0
31	HP19	0	0	0	0
32	HP20	0	0	0	0
33	HP21	0	0	0	0
34	HP22	0	0	0	0
35	HP23	0	0	0	0
36	HP24	0	0	0	0
37	HP25	0	0	0	0
38	HP26	0	0	0	0
39	HP27	0	0	0	0
40	HP28	0	0	0	0
41	HP29	0	0	0	0
42	HP30	0	0	0	0
43	HP31	0	0	0	0
44	HP32	0	0	0	0
45	F1.1_td	0	0	0	0
46	F1.2_td	0	1	0	1
47	F1.3_td	0	0	0	0
48	F1.4_td	0	0	0	0
49	F2.1_td	0	0	0	0
50	F2.2_td	0	0	0	0
51	F2.3_td	0	0	0	0
52	F2.4_td	0	0	0	0
53	F3.1_td	0	0	0	0
54	F3.2_td	0	0	0	0
55	F3.3_td	0	0	0	0
56	F3.4_td	0	0	0	0
57	F4.1_td	0	0	0	0
58	F4.2_td	0	0	0	0
59	F4.3_td	0	0	0	0
60	F4.4_td	0	0	0	0
61	F5.1_td	0	0	0	0
62	F5.2_td	0	0	0	0
63	F5.3_td	0	0	0	0
64	F5.4_td	0	0	0	0
65	F6.1_td	0	0	0	0
66	F6.2_td	0	0	0	0
67	F6.3_td	0	0	0	0
68	F6.4_td	0	0	0	0
69	F09~WGA	1	0	1	1
70	F10~WGA	1	0	1	1
71	F11~1ng/mkl	1	1	0	1
72	F12~1ng/mkl	1	1	0	1
73	G01~100ng/mkl	1	1	0	1
74	G02~100ng/mkl	1	1	0	1
75	G03~1ng/mkl	0	0	0	0
76	G04~1ng/mkl	0	0	0	0
77	G05~100ng/mkl	0	0	0	0
78	G06~100ng/mkl	0	0	0	0
79	G07~1ng/mkl	1	1	0	1
80	G08~1ng/mkl	1	1	0	1
81	G09~100ng/mkl	1	1	0	1
82	G10~100ng/mkl	1	1	0	1
83	G11~1ng/mkl	0	0	0	0
84	G12~1ng/mkl	0	0	0	0
85	H01~100ng/mkl	0	0	0	0
86	H02~100ng/mkl	0	0	0	0
87	s1	1	1	0	1
88	s2	1	1	0	1
89	s3	1	1	0	1
90	s4	1	1	0	1
91	s5	1	1	0	1
92	s6	1	1	1	1
93	s7	0	0	0	0
94	s8	1	1	0	1
95	NTC	0	1	0	1
96	NTC	0	0	0	0

2 Performance analysis

The performance of the **hookreg()** function and **hookregNL()** function was analyzed with the **performeR()** function of the `PCRedux` package. The methods were adopted from Brenner and Gefeller (1997) and Kuhn (2008).

```r
res_performeR <- rbind(
  hookreg=performeR(res_out[["hookreg"]], res_out[["Human rater"]]),
  hookregNL=performeR(res_out[["hookregNL"]], res_out[["Human rater"]]),
  combined_hookreg=performeR(res_out[["hookreg and hoohkreNL combined"]],
                            res_out[["Human rater"]])
) %>% t %>% signif(4)

colnames(res_performeR) <- c("hookreg", "hookregNL", "hookreg and hookregNL")
```

```r
library(xtable)
options(xtable.comment=FALSE)

print(xtable(res_performeR, digits=0),
      size = "normalsize",
      include.rownames = TRUE,
      include.colnames = TRUE,
      caption.placement = "top",
      comment=FALSE,
      table.placement = "!ht", scalebox='0.75', floating=FALSE
)
```

	hookreg	hookregNL	hookreg and hookregNL
TPR	1	0	1
SPC	1	1	1
PPV	1	1	1
NPV	1	1	1
FPR	0	0	0
FNR	0	1	0
FDR	0	0	0
ACC	1	1	1
F1	1	0	1
MCC	1	1	1
LRp	34	Inf	38
kappa	1	0	1
TP	19	7	21
TN	73	75	73
FP	2	0	2
FN	2	14	0
counts	96	96	96

3 Hook effect analysis with rdmlEdit GUI

One can analyze data with GUI by installing `RDML` package and run **rdmlEdit** as local server, or open rdmlEdit app at Evrogen server. After opening **rdmlEdit** you can see several tabs at the top of the screen. Inside *Files* tab click *Browse. . .* button to select your file. After, the file is opened you can see its structure at right of the screen presented as dendrogramm.

Click to the `qPCR` tab to start analysis. Select a hook detection method at *Hook Detection Method* selector and wait for analysis. Results can be viewed inside the table (*hook* column) or by color and shape of PCR curves (select *Hook* at *Color by* and *Line Type by* selectors).

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