

Package: RDML (via r-universe)

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Type Package

Title Importing Real-Time Thermo Cyclers (qPCR) Data from RDML Format Files

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Description Imports real-time thermo cyclers (qPCR) data from Real-time PCR Data Markup Language (RDML) and transforms to the appropriate formats of the 'qpcR' and 'chipPCR' packages. Contains a dendrogram visualization for the structure of RDML object and GUI for RDML editing.

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URL <https://github.com/PCRuniversum/RDML>

Depends R (>= 3.2.0)

Imports checkmate (>= 1.6.2), data.table, pipeR, readxl, rlist (>= 0.4), R6 (>= 2.0.1), stringr, tools (>= 3.2), xml2 (>= 1.0), lubridate (>= 1.6.0)

Collate 'RDML.types.R' 'RDML.R' 'RDML.AsDendrogram.R' 'RDML.AsTable.R' 'RDML.GetFDData.R' 'RDML.Merge.R' 'RDML.SetFDData.R' 'RDML.init.R' 'functional_wrappers.R' 'rdmlEdit.R'

Suggests chipPCR, magrittr, reshape2, qpcR, dplyr, ggplot2, knitr, kfigr, MBmca, shiny, shinyjs, shinythemes, shinyMolBio, V8, testthat

RoxygenNote 7.3.1

Repository <https://pcruniversum.r-universe.dev>

RemoteUrl <https://github.com/pcruniversum/rdml>

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Contents

adpsType	3
annotationType	5
as.character.idType	6
as.character.reactIdType	6
AsDendrogram	7
AsTable	7
baseTemperatureType	8
cdnaSynthesisMethodType	9
commercialAssayType	10
cqDetectionMethodType	11
dataCollectionSoftwareType	12
dataType	13
documentationType	14
dyeType	15
enumType	16
experimenterType	17
experimentType	19
GetFData	20
gradientType	20
idReferencesType	21
idType	22
labelFormatType	23
lidOpenType	24
loopType	25
mdpsType	26
measureType	27
MergeRDMLs	28
new	28
nucleotideType	29
oligoType	30
pauseType	31
pcrFormatType	32
primingMethodType	33
quantityType	34
quantityUnitType	35
RDML	36
RDML.AsDendrogram	41
RDML.AsTable	42
RDML.GetFData	43
RDML.SetFData	44
rdmlBaseType	45
rdmlEdit	46
rdmlIdType	47
reactIdType	48
reactType	49
runType	51

sampleType	53
sampleTypeType	54
sequencesType	55
SetFData	57
stepType	57
targetType	58
targetTypeType	60
temperatureType	61
templateQuantityType	62
thermalCyclingConditionsType	63
xRefType	64
[.GetFData	65

Index	66
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adpsType	<i>adpsType R6 class.</i>
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Description

adpsType R6 class.

adpsType R6 class.

Format

An [R6Class](#) generator object.

Details

Contains matrix of amplification data. Must have three columns:

cyc PCR cycle at which data point was collected (every cycle must have unique number).

tmp temperature in degrees Celsius at the time of measurement (optional).

fluor raw fluorescence intensity measured.

Inherits: [rdmlBaseType](#).

Initialization

```
adpsType$new(fpoints)
```

Fields

fpoints [assertMatrix](#). Matrix with amplification data points.

Super class

[RDML::rdmlBaseType](#) -> adpsType

Methods

Public methods:

- [adpsType\\$new\(\)](#)
- [adpsType\\$.asXMLnodes\(\)](#)
- [adpsType\\$clone\(\)](#)

Method new():

Usage:

```
adpsType$new(fpoints)
```

Method .asXMLnodes():

Usage:

```
adpsType$.asXMLnodes(node.name)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
adpsType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
#cycles
cyc <- c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17,
18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33,
34, 35, 36, 37, 38, 39, 40)
#fluorescence
fluo <- c(2.0172, 2.0131, 2.0035, 2, 2.0024, 2.0056, 2.0105, 2.0179,
2.0272, 2.0488, 2.0922, 2.1925, 2.3937, 2.7499, 3.3072, 4.0966,
5.0637, 6.0621, 7.0239, 7.8457, 8.5449, 9.1282, 9.6022, 9.9995,
10.2657, 10.4989, 10.6813, 10.8209, 10.9158, 10.9668, 11.0053,
11.0318, 11.0446, 11.044, 11.0052, 10.9671, 10.9365, 10.9199,
10.897, 10.8316)
#temperature
temp <- c(55, 55, 55, 55, 54, 54, 55, 55, 55, 55, 55, 55, 55, 55, 55,
55, 55, 55, 55, 55, 55, 55, 55, 56, 55, 55, 55, 55, 55, 55,
55, 55, 55, 55, 55, 55, 55, 55)

#combine all variables into a proper object
data <- data.frame(cyc = cyc, tmp = temp, fluor = fluo)

#create adps object
adpsType$new(data)

#create adps object without temperature data
adpsType$new(data[, -2])
```

annotationType	<i>annotationType R6 class.</i>
----------------	---------------------------------

Description

Annotate samples by setting a property and its value. For example, sex could be a property with the possible values M or F. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Fields

property [checkString](#). Property name

value [checkString](#). Value

Super class

[RDML::rdmlBaseType](#) -> annotationType

Methods

Public methods:

- [annotationType\\$new\(\)](#)
- [annotationType\\$clone\(\)](#)

Method new():

Usage:

```
annotationType$new(property, value)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
annotationType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
#set sex property
annotationType$new(property = "sex", value = "M")
```

as.character.idType *Convert idType object to character*

Description

Function to convert idType object to character.

Usage

```
## S3 method for class 'idType'  
as.character(x, ...)
```

Arguments

x idType object.
... Further arguments to be passed.

as.character.reactIdType
 Convert reactIdType object to character

Description

Function to convert reactIdType object to character.

Usage

```
## S3 method for class 'reactIdType'  
as.character(x, ...)
```

Arguments

x reactIdType object.
... Further arguments to be passed.

AsDendrogram	RDML\$AsDendrogram() <i>wrapper</i>
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Description

Read more at [RDML.AsDendrogram](#)

Usage

```
AsDendrogram(obj, ...)
```

Arguments

obj	RDML object.
...	AsDendrogram params.

AsTable	RDML\$AsTable() <i>wrapper</i>
---------	--------------------------------

Description

Read more at [RDML.AsTable](#)

Usage

```
AsTable(obj, ...)
```

Arguments

obj	RDML object.
...	AsTable params.

baseTemperatureType *baseTemperatureType R6 class.*

Description

Parent class for inner usage. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
baseTemperatureType$new(duration,
  temperatureChange = NULL, durationChange = NULL, measure = NULL, ramp =
  NULL)
```

Fields

duration [checkCount](#). Duration of this step in seconds.

temperatureChange [checkNumber](#). Change of the temperature between two consecutive cycles:
actual temperature = temperature + (temperatureChange * cycle counter)

durationChange [checkCount](#). Change of the duration between two consecutive cycles: actual
duration = duration + (durationChange * cycle counter)

measure [measureType](#). Indicates to make a measurement and store it as meltcurve or real-time
data.

ramp [checkNumber](#). Allowed temperature change between two consecutive cycles in degrees Cel-
sius per second. If unstated, the maximal change rate is assumed.

Super class

[RDML::rdmlBaseType](#) -> baseTemperatureType

Methods

Public methods:

- [baseTemperatureType\\$new\(\)](#)
- [baseTemperatureType\\$clone\(\)](#)

Method new():

Usage:

```
baseTemperatureType$new(
  duration,
  temperatureChange = NULL,
  durationChange = NULL,
  measure = NULL,
```



```

        ramp = NULL
    )

```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
baseTemperatureType$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

cdnaSynthesisMethodType

cdnaSynthesisMethodType R6 class.

Description

Description of the cDNA synthesis method. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
cdnaSynthesisMethodType$new(enzyme = NULL,
  primingMethod = NULL, dnaseTreatment = NULL, thermalCyclingConditions =
  NULL)
```

@section Fields:

`enzyme` [checkString](#). Name of the enzyme used for reverse transcription.

`primingMethod` [primingMethodType](#).

`dnaseTreatment` [checkFlag](#) if TRUE RNA was DNase treated prior cDNA synthesis.

`thermalCyclingConditions` [idReferencesType](#).

Super class

[RDML::rdmlBaseType](#) -> [cdnaSynthesisMethodType](#)

Methods

Public methods:

- [cdnaSynthesisMethodType\\$new\(\)](#)
- [cdnaSynthesisMethodType\\$clone\(\)](#)

Method `new()`:

Usage:

```

cdnaSynthesisMethodType$new(
  enzyme = NULL,
  primingMethod = NULL,
  dnaseTreatment = NULL,
  thermalCyclingConditions = NULL
)

```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
cdnaSynthesisMethodType$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

commercialAssayType *commercialAssayType R6 class.*

Description

For some commercial assays, the primer sequences may be unknown. This element allows to describe commercial assays. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
commercialAssayType$new(company, orderNumber)
```

@section Fields:

`company` [checkString](#).

`orderNumber` [checkString](#).

Super class

[RDML::rdmlBaseType](#) -> commercialAssayType

Methods

Public methods:

- [commercialAssayType\\$new\(\)](#)
- [commercialAssayType\\$clone\(\)](#)

Method `new()`:

Usage:

```
commercialAssayType$new(company, orderNumber)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
commercialAssayType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

cqDetectionMethodType *cqDetectionMethodType R6 class.*

Description

The method used to determine the Cq value. Can take values:

"automated threshold and baseline settings"

"manual threshold and baseline settings"

"second derivative maximum"

"other"

Inherits: [enumType](#).

Format

An [R6Class](#) generator object.

Initialization

```
cqDetectionMethodType$new(value)
```

@section Fields:

value [checkString](#).

Super classes

```
RDML::rdmlBaseType -> RDML::enumType -> cqDetectionMethodType
```

Methods

Public methods:

- [cqDetectionMethodType\\$clone\(\)](#)

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
cqDetectionMethodType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

dataCollectionSoftwareType
dataCollectionSoftwareType R6 class.

Description

Software name and version used to collect and analyze the data. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
dataCollectionSoftwareType$new(name, version)
```

@section Fields:

name [checkString](#).

version [checkString](#).

Super class

```
RDML::rdmlBaseType -> dataCollectionSoftwareType
```

Methods

Public methods:

- [dataCollectionSoftwareType\\$new\(\)](#)
- [dataCollectionSoftwareType\\$clone\(\)](#)

Method new():

Usage:

```
dataCollectionSoftwareType$new(name, version)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
dataCollectionSoftwareType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
dataCollectionSoftwareType$new(name = "ExampleSoft",  
                               version = "1.0")
```

dataType	<i>dataType R6 class.</i>
----------	---------------------------

Description

Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
dataType$new(tar, cq = NULL, excl = NULL,
adp = NULL, mdp = NULL, endPt = NULL, bgFluor = NULL, bgFluorSlp = NULL,
quantFluor = NULL)
```

Fields

tar [idReferencesType](#). TargetID - A reference to a target.

cq [checkNumber](#). Calculated fractional PCR cycle used for downstream quantification. Negative values express following condition: Not Available: -1.0 . (can be NaN for BioRad Maestro compatibility)

excl [checkString](#). Excluded. If excl is present, this entry should not be evaluated. Do not set this element to FALSE if the entry is valid. Instead, leave the entire excl element out instead. It may contain a string with a reason for the exclusion. Several reasons for exclusion should be separated by semicolons ";".

adp [adpsType](#).

mdp [mdpsType](#).

endPt [checkNumber](#). Value of the endpoint measurement.

bgFluor [checkNumber](#). Background fluorescence (the y-intercept of the baseline trend based on the estimated background fluorescence).

bgFluorSlp [checkNumber](#). Background fluorescence slope - The slope of the baseline trend based on the estimated background fluorescence. The element should be absent to indicate a slope of 0.0; If this element is present without the bgFluor element it should be ignored.

quantFluor [checkNumber](#). Quantification fluorescence - The fluorescence value corresponding to the threshold line.

Methods

```
AsDataFrame(dp.type = "adp") Represents amplification (
  dp.type = "adp"
) or melting (dp.type = "mdp") data points as data.frame
```

Super class

`RDML::rdmlBaseType` -> dataType

Methods**Public methods:**

- `dataType$new()`
- `dataType$GetFDData()`
- `dataType$clone()`

Method new():

Usage:

```
dataType$new(  
  tar,  
  cq = NULL,  
  excl = NULL,  
  adp = NULL,  
  mdp = NULL,  
  endPt = NULL,  
  bgFluor = NULL,  
  bgFluorSlp = NULL,  
  quantFluor = NULL  
)
```

Method GetFDData():

Usage:

```
dataType$GetFDData(dp.type = "adp")
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
dataType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

documentationType *documentationType R6 class.*

Description

These elements should be used if the same description applies to many samples, targets or experiments. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
documentationType$new(id, text = NULL)
```

@section Fields:

id [idType](#). Identifier.

text [checkString](#). Text.

Super class

```
RDML::rdmlBaseType -> documentationType
```

Methods**Public methods:**

- [documentationType\\$new\(\)](#)
- [documentationType\\$clone\(\)](#)

Method new():

Usage:

```
documentationType$new(id, text = NULL)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
documentationType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

dyeType

dyeType R6 class.

Description

Detailed information about the dye. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
dyeType$new(id, description = NULL)
```

@section Fields:

id [idType](#). Identifier.

description [checkString](#). Description.

Super class

[RDML::rdmlBaseType](#) -> dyeType

Methods**Public methods:**

- [dyeType\\$new\(\)](#)
- [dyeType\\$clone\(\)](#)

Method new():

Usage:

```
dyeType$new(id, description = NULL)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
dyeType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

enumType

enumType R6 class.

Description

Generic class for creating objects that can take limited list of values.

Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
enumType$new(value)
```

@section Fields:

value [checkString](#). Value.

Super class

[RDML::rdmlBaseType](#) -> enumType

Methods

Public methods:

- [enumType\\$new\(\)](#)
- [enumType\\$print\(\)](#)
- [enumType\\$.asXMLnodes\(\)](#)
- [enumType\\$clone\(\)](#)

Method new():

Usage:

```
enumType$new(value)
```

Method print():

Usage:

```
enumType$print(...)
```

Method .asXMLnodes():

Usage:

```
enumType$.asXMLnodes(node.name)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
enumType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

experimenterType *experimenterType R6 class.*

Description

Contact details of the experimenter. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
experimenterType$new(id, firstName, lastName,  
  email = NULL, labName = NULL, labAddress = NULL)
```

@section Fields:

id `idType`. Identifier.

firstName `checkString`. First name.

lastName `checkString`. Last name.

email `checkString`. Email.

labName `checkString`. Lab name.

labAddress `checkString`. Lab address.

Super class

```
RDML::rdmlBaseType -> experimenterType
```

Methods**Public methods:**

- `experimenterType$new()`
- `experimenterType$clone()`

Method new():

Usage:

```
experimenterType$new(  
  id,  
  firstName,  
  lastName,  
  email = NULL,  
  labName = NULL,  
  labAddress = NULL  
)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
experimenterType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

experimentType	<i>experimentType R6 class.</i>
----------------	---------------------------------

Description

A qPCR experiment. It may contain several runs ([runType](#)). Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
experimentType$new(id, description = NULL,
  documentation = NULL, run = NULL)
```

@section Fields:

id [idType](#).

description [checkString](#).

documentation list of [idReferencesType](#).

run list of [runType](#).

Methods

`AsDataFrame(dp.type = "adp", long.table = FALSE)` Represents amplification (`dp.type = "adp"`) or melting (`dp.type = "mdp"`) data points as `data.frame`. `long.table = TRUE` means that fluorescence data for all runs and reacts will be at one column.

Super class

`RDML::rdmlBaseType -> experimentType`

Methods**Public methods:**

- [experimentType\\$new\(\)](#)
- [experimentType\\$GetFData\(\)](#)
- [experimentType\\$clone\(\)](#)

Method new():

Usage:

```
experimentType$new(id, description = NULL, documentation = NULL, run = NULL)
```

Method GetFData():

Usage:

```
experimentType$GetFData(dp.type = "adp", long.table = FALSE)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
experimentType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

GetFData	RDML\$GetFData() <i>wrapper</i>
----------	---------------------------------

Description

Read more at [RDML.GetFData](#)

Usage

```
GetFData(obj, ...)
```

Arguments

obj	RDML object.
...	GetFData params.

gradientType	<i>gradientType R6 class.</i>
--------------	-------------------------------

Description

Details of the temperature gradient across the PCR block. Inherits: [baseTemperatureType](#).

Format

An [R6Class](#) generator object.

Initialization

```
gradientType$new(highTemperature,  
  lowTemperature, ...)
```

Fields

highTemperature [checkNumber](#). The highest temperature of the gradient in degrees Celsius.
 lowTemperature [checkNumber](#). The lowest temperature of the gradient in degrees Celsius.
 ... Params of parent class [baseTemperatureType](#).

Super classes

`RDML::rdmlBaseType -> RDML::baseTemperatureType -> gradientType`

Methods

Public methods:

- `gradientType$new()`
- `gradientType$clone()`

Method new():

Usage:

`gradientType$new(highTemperature, lowTemperature, ...)`

Method clone(): The objects of this class are cloneable with this method.

Usage:

`gradientType$clone(deep = FALSE)`

Arguments:

`deep` Whether to make a deep clone.

`idReferencesType` *idReferencesType R6 class.*

Description

Contains id of another RDML object. Inherits: [idType](#).

Format

An [R6Class](#) generator object.

Initialization

`idReferencesType$new(id)`

Fields

`id` [checkString](#). Identifier.

Super classes

`RDML::rdmlBaseType -> RDML::idType -> idReferencesType`

Methods**Public methods:**

- [idReferencesType\\$clone\(\)](#)

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
idReferencesType$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

idType

idType R6 class.

Description

Contains identifier for various RDML types. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
idType$new(id)
```

@section Fields:

`id` [checkString](#). Identifier.

Super class

```
RDML::rdmlBaseType -> idType
```

Methods**Public methods:**

- [idType\\$new\(\)](#)
- [idType\\$.asXMLnodes\(\)](#)
- [idType\\$clone\(\)](#)

Method `new()`:

Usage:

```
idType$new(id)
```

Method `.asXMLnodes()`:

Usage:

```
idType$.asXMLnodes(node.name)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
idType$.clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

labelFormatType

labelFormatType R6 class.

Description

Label used for [pcrFormatType](#). Can take values:

ABC

123

A1a1

Inherits: [enumType](#).

Format

An [R6Class](#) generator object.

Initialization

```
labelFormatType$new(value)
```

@section Fields:

value [checkString](#).

Super classes

```
RDML::rdmlBaseType -> RDML::enumType -> labelFormatType
```

Methods

Public methods:

- [labelFormatType\\$.clone\(\)](#)

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
labelFormatType$.clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

lidOpenType	<i>lidOpenType R6 class.</i>
-------------	------------------------------

Description

This step waits for the user to open the lid and continues afterwards. It allows to stop the program and to wait for the user to add for example enzymes and continue the program afterwards. The temperature of the previous step is maintained. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
lidOpenType$new()
```

Super class

```
RDML::rdmlBaseType -> lidOpenType
```

Methods

Public methods:

- [lidOpenType\\$new\(\)](#)
- [lidOpenType\\$clone\(\)](#)

Method new():

Usage:

```
lidOpenType$new()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
lidOpenType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

loopType	<i>loopType R6 class.</i>
----------	---------------------------

Description

This step allows to form a loop or to exclude some steps. It allows to jump to a certain "goto" step for "repeat" times. If the "goto" step is outside of the loop range, it must have "repeat" value "0". Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
loopType$new(goto, repeat.n)
```

Fields

goto [assertCount](#). The step to go to to form the loop.

repeat.n [assertCount](#). Determines how many times the loop is repeated. The first run through the loop is counted as 0, the last loop is "repeat" - 1.

Super class

```
RDML::rdmlBaseType -> loopType
```

Methods

Public methods:

- [loopType\\$new\(\)](#)
- [loopType\\$clone\(\)](#)

Method new():

Usage:

```
loopType$new(goto, repeat.n)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
loopType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

mdpsType

mdpsType R6 class.

Description

Contains matrix of melting data points (single data points measured during amplification).

Format

An [R6Class](#) generator object.

Details

Columns:

tmp (temperature in degrees Celsius at the time of measurement. Every point must have unique value.

fluor fluorescence intensity measured without any correction (including baselining).

Inherits: [rdmlBaseType](#).

Initialization

`mdpsType$new(fpoints)`

@section Fields:

`fpoints` [assertMatrix](#). Matrix with amplification data points.

Super class

`RDML::rdmlBaseType -> mdpsType`

Methods

Public methods:

- `mdpsType$new()`
- `mdpsType$.asXMLnodes()`
- `mdpsType$clone()`

Method `new()`:

Usage:

`mdpsType$new(fpoints)`

Method `.asXMLnodes()`:

Usage:

`mdpsType$.asXMLnodes(node.name)`

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
mdpsType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

measureType

measureType R6 class.

Description

Can take values:

real time

meltcurve

Inherits: [enumType](#).

Format

An [R6Class](#) generator object.

Initialization

```
measureType$new(value)
```

@section Fields:

value [checkString](#).

Super classes

```
RDML::rdmlBaseType -> RDML::enumType -> measureType
```

Methods

Public methods:

- [measureType\\$clone\(\)](#)

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
measureType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

MergeRDMLs

Merges RDML objects

Description

Merges list of RDML objects. The first object in the list becomes base object. If experiments or runs have same name they will be combined. Reacts with same id, experiment and run overwrite each other!

Usage

```
MergeRDMLs(to.merge)
```

Arguments

to.merge RDML objects that should be merged.

Examples

```
## Not run:
PATH <- path.package("RDML")
filename <- paste(PATH, "/extdata/", "lc96_bACTXY.rdm1", sep = "")
lc96 <- RDML$new(filename)
filename <- paste(PATH, "/extdata/", "stepone_std.rdm1", sep = "")
stepone <- RDML$new(filename)
merged <- MergeRDMLs(list(lc96,stepone))
merged$AsDendrogram()

## End(Not run)
```

new

Creates new instance of RDML class object

Description

This function has been designed to import data from RDML v1.1 and v1.2 format files or from xls file generated by *Applied Biosystems 7500*. To import from xls this file have to contain Sample Setup and Multicomponent Data sheets!

Arguments

filename string – path to file
show.progress logical – show loading progress bar if TRUE
conditions.sep separator for condition defined at sample name
format string – input file format. Possible values auto, rdml, abi, excel, csv. See Details.

Details

File format options:

- auto** Tries to detect format by extension. `.xlsx` – excel, `.xls` – abi, `.csv` – csv, other – rdml
- abi** Reads `.xls` files generated by *ABI 7500 v.2*. To create such files use File>Export; check 'Sample Setup' and 'Multicomponent Data'; select 'One File'
- excel** `.xls` or `.xlsx` file with sheets 'description', 'adp', 'mdp'. See example file `table.xlsx`
- csv** `.csv` file with first column 'cyc' or 'tmp' and fluorescence data in other columns
- rdml** `.rdml` or `.lc96p` files

Warning

Although the format RDML claimed as data exchange format, the specific implementation of the format at devices from real manufacturers differ significantly. Currently this function is checked against RDML data from devices: *Bio-Rad CFX96*, *Roche LightCycler 96* and *Applied Biosystems StepOne*.

Author(s)

Konstantin A. Blagodatskikh <k.blag@yandex.ru>, Stefan Roediger <stefan.roediger@b-tu.de>, Michal Burdukiewicz <michalburdukiewicz@gmail.com>

Examples

```
## Not run:
## Import from RDML file
PATH <- path.package("RDML")
filename <- paste(PATH, "/extdata/", "lc96_bACTXY.rdml", sep = "")
lc96 <- RDML$new(filename)

## Some kind of overview for lc96
lc96$AsTable(name.pattern = sample[[react$sample$id]]$description)
lc96$AsDendrogram()

## End(Not run)
```

nucleotideType

nucleotideType R6 class.

Description

Type of nucleic acid used as a template in the experiment. May have following values:

DNA
genomic DNA
cDNA
RNA

Format

An [R6Class](#) generator object.

Details

Inherits: [enumType](#).

Initialization

```
nucleotideType$new(value)
```

@section Fields:

value [checkString](#). Value.

Super classes

```
RDML::rdmlBaseType -> RDML::enumType -> nucleotideType
```

Methods**Public methods:**

- [nucleotideType\\$clone\(\)](#)

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
nucleotideType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

oligoType

oligoType R6 class.

Description

Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
oligoType$new(threePrimeTag = NULL,
              fivePrimeTag = NULL, sequence)
```

@section Fields:

threePrimeTag [checkString](#). Description of three prime modification (if present).

fivePrimeTag [checkString](#). Description of five prime modification (if present).

sequence [checkString](#).

Super class

[RDML::rdmlBaseType](#) -> oligoType

Methods**Public methods:**

- [oligoType\\$new\(\)](#)
- [oligoType\\$clone\(\)](#)

Method new():

Usage:

`oligoType$new(threePrimeTag = NULL, fivePrimeTag = NULL, sequence)`

Method clone(): The objects of this class are cloneable with this method.

Usage:

`oligoType$clone(deep = FALSE)`

Arguments:

deep Whether to make a deep clone.

pauseType

pauseType R6 class.

Description

This step allows to pause at a certain temperature. It is typically the last step in an amplification protocol. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

`pauseType$new(temperature)`

Fields

temperature [checkNumber](#). The temperature in degrees Celsius maintained during the pause.

Super class

[RDML::rdmlBaseType](#) -> pauseType

Methods**Public methods:**

- [pauseType\\$new\(\)](#)
- [pauseType\\$clone\(\)](#)

Method new():*Usage:*

pauseType\$new(temperature)

Method clone(): The objects of this class are cloneable with this method.*Usage:*

pauseType\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

pcrFormatType *pcrFormatType R6 class.*

Description

The display format of the PCR, analogous to the the qPCR instrument run format. Inherits: [rdml-BaseType](#).

Format

An [R6Class](#) generator object.

Details

Rotor formats always have 1 column; rows correspond to the number of places in the rotor. Values for common formats are:

Format	rows	columns	rowLabel	columnLabel
single-well	1	1	123	123
48-well plate	6	8	ABC	123
96-well plate	8	12	ABC	123
384-well plate	16	24	ABC	123
1536-well plate	32	48	ABC	123
3072-well array	32	96	A1a1	A1a1
5184-well chip	72	72	ABC	123
32-well rotor	32	1	123	123
72-well rotor	72	1	123	123
100-well rotor	100	1	123	123
free format	-1	1	123	123

If rows field has value -1, the function will not try to reconstruct a plate and just display all run data in a single column. If the columns field has value 1 then the function will not display a column label.

Initialization

```
pcrFormatType$new(rows, columns, rowLabel, columnLabel)
```

@section Fields:

rows [checkCount](#).

columns [checkCount](#).

rowLabel [labelFormatType](#).

columnLabel [labelFormatType](#).

Super class

```
RDML::rdmlBaseType -> pcrFormatType
```

Methods**Public methods:**

- [pcrFormatType\\$new\(\)](#)
- [pcrFormatType\\$clone\(\)](#)

Method new():

Usage:

```
pcrFormatType$new(rows, columns, rowLabel, columnLabel)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
pcrFormatType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

primingMethodType *primingMethodType R6 class.*

Description

The primers used in the reverse transcription. Can take values:

oligo-dt

random

target-specific

oligo-dt and random

other

Format

An [R6Class](#) generator object.

Details

Inherits: [enumType](#).

Initialization

```
primingMethodType$new(value)
```

@section Fields:

value [checkString](#). Value.

Super classes

```
RDML::rdmlBaseType -> RDML::enumType -> primingMethodType
```

Methods**Public methods:**

- [primingMethodType\\$clone\(\)](#)

Method [clone\(\)](#): The objects of this class are cloneable with this method.

Usage:

```
primingMethodType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

quantityType

quantityType R6 class.

Description

A quantity is always defined by its value and its unit. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
quantityType$new(value, unit)
```

@section Fields:

value [checkNumber](#). Value.

unit [quantityUnitType](#). Unit.

Super class

`RDML::rdmlBaseType` -> quantityType

Methods**Public methods:**

- `quantityType$new()`
- `quantityType$clone()`

Method new():

Usage:

`quantityType$new(value, unit)`

Method clone(): The objects of this class are cloneable with this method.

Usage:

`quantityType$clone(deep = FALSE)`

Arguments:

`deep` Whether to make a deep clone.

quantityUnitType *quantityUnitType R6 class.*

Description

The unit the quantity. Can take values:

cop copies per microliter

fold fold change

dil dilution (10 would mean 1:10 dilution)

nMol nanomol per microliter

ng nanogram per microliter

other other unit (must be linear, no exponents or logarithms allowed)

Format

An `R6Class` generator object.

Details

Inherits: `enumType`.

Initialization

```
quantityUnitType$new(value)
```

@section Fields:

value [checkString](#). Value.

Super classes

```
RDML::rdmlBaseType -> RDML::enumType -> quantityUnitType
```

Methods**Public methods:**

- [quantityUnitType\\$clone\(\)](#)

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
quantityUnitType$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

RDML

R6 class RDML – contains methods to read and overview fluorescence data from RDML v1.1 and v1.2 format files

Description

This class is a container for RDML format data (Lefever et al. 2009). The data may be further transformed to the appropriate format of the `qpcR` (Ritz et al. 2008, Spiess et al. 2008) and `chipPCR` (Roediger et al. 2015) packages (see [RDML.new](#) for import details). Real-time PCR Data Markup Language (RDML) is the recommended file format element in the Minimum Information for Publication of Quantitative Real-Time PCR Experiments (MIQE) guidelines (Bustin et al. 2009). The inner structure of imported data faithfully reflects the structure of RDML file v1.2. All data with the exception for fluorescence values can be represented as `data.frame` by method `AsTable`. Such possibility of data representation streamlines sample filtering (by targets, types, etc.) and serves as request for `GetFData` method, which extracts fluorescence data for specified samples.

Format

An [R6Class](#) generator object.

Fields

Type, structure of data and description of fields can be viewed at RDML v1.2 file description. Names of fields are first level of XML tree.

Methods

new creates a new instance of RDML class object (see [RDML.new](#))

AsTable represent RDML data as data.frame (see [RDML.AsTable](#))

GetFData gets fluorescence data (see [RDML.GetFData](#))

SetFData sets fluorescence data (see [RDML.SetFData](#))

Merge merges two RDML to one (see [MergeRDMLs](#))

AsDendrogram represents structure of RDML object as dendrogram(see [RDML.AsDendrogram](#))

Super class

[RDML::rdmlBaseType](#) -> RDML

Methods**Public methods:**

- [RDML\\$AsDendrogram\(\)](#)
- [RDML\\$AsTable\(\)](#)
- [RDML\\$GetFData\(\)](#)
- [RDML\\$AsXML\(\)](#)
- [RDML\\$SetFData\(\)](#)
- [RDML\\$new\(\)](#)
- [RDML\\$clone\(\)](#)

Method `AsDendrogram()`:

Usage:

```
RDML$AsDendrogram(plot.dendrogram = TRUE)
```

Method `AsTable()`:

Usage:

```
RDML$AsTable(
  .default = list(exp.id = experiment$id$id, run.id = run$id$id, react.id = react$id$id,
    position = react$position, sample = react$sample$id, target = data$star$id,
    target.dyeId = target[[data$star$id]]$dyeId$id, sample.type =
    sample[[react$sample$id]]$type$value, adp = !is.null(data$adp), mdp =
    !is.null(data$mdp)),
  name.pattern = paste(react$position, react$sample$id,
    private$.sample[[react$sample$id]]$type$value, data$star$id, sep = "_"),
  add.columns = list(),
  treat.null.as.na = FALSE,
  ...
)
```

Method `GetFData()`:

Usage:

```
RDML$GetFData(request, dp.type = "adp", long.table = FALSE)
```

Method AsXML():*Usage:*

RDML\$AsXML(file.name)

Method SetFData():*Usage:*

RDML\$SetFData(fdata, description, fdata.type = "adp")

Method new():*Usage:*

```
RDML$new(
  filename,
  show.progress = TRUE,
  conditions.sep = NULL,
  cluster = NULL,
  format = "auto"
)
```

Method clone(): The objects of this class are cloneable with this method.*Usage:*

RDML\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Author(s)

Konstantin A. Blagodatskikh <k.blag@yandex.ru>, Stefan Roediger <stefan.roediger@b-tu.de>, Michal Burdukiewicz <michalburdukiewicz@gmail.com>

References

RDML format <http://www.rdml.org/> R6 package <http://cran.r-project.org/web/packages/R6/index.html>

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Examples

```

## EXAMPLE 1:
## internal dataset lc96_bACTXY.rdml (in 'data' directory)
## generated by Roche LightCycler 96. Contains qPCR data
## with four targets and two types.
## Import with default settings.
PATH <- path.package("RDML")
filename <- paste(PATH, "/extdata/", "lc96_bACTXY.rdml", sep = "")
lc96 <- RDML$new(filename)

tab <- lc96$AsTable(name.pattern = paste(sample[[react$sample$id]]$description,
                                       react$id$id),
                  quantity = sample[[react$sample$id]]$quantity$value)

## Show dyes names
unique(tab$target.dyeId)
## Show types of the samples for dye 'FAM'
library(dplyr)
unique(filter(tab, target.dyeId == "FAM")$sample.type)

## Show template quantities for dye 'FAM' type 'std'#
## Not run:
COPIES <- filter(tab, target.dyeId == "FAM", sample.type == "std")$quantity
## Define calibration curves (type of the samples - 'std').
## No replicates.
library(qpcR)
CAL <- modlist(lc96$GetFData(filter(tab,
                                   target.dyeId == "FAM",
                                   sample.type == "std")),
              baseline="lin", basecyc=8:15)
## Define samples to predict (first two samples with the type - 'unkn').
PRED <- modlist(lc96$GetFData(filter(tab,
                                   target.dyeId == "FAM",
                                   sample.type == "unkn")),
              baseline="lin", basecyc=8:15)

## Conduct quantification.
calib(refcurve = CAL, predcurve = PRED, thresh = "cpD2",
      dil = COPIES)

## End(Not run)
## Not run:
## EXAMPLE 2:
## internal dataset lc96_bACTXY.rdml (in 'data' directory)
## generated by Roche LightCycler 96. Contains qPCR data
## with four targets and two types.
## Import with default settings.
library(chipPCR)
PATH <- path.package("RDML")
filename <- paste(PATH, "/extdata/", "lc96_bACTXY.rdml", sep = "")
lc96 <- RDML$new(filename)

tab <- lc96$AsTable(name.pattern = paste(sample[[react$sample$id]]$description,
                                       react$id$id),

```

```

        quantity = sample[[react$sample$id]]$quantity$value)
## Show targets names
unique(tab$target)
## Fetch cycle dependent fluorescence for HEX channel
tmp <- lc96$GetFDData(filter(tab, target == "bACT", sample.type == "std"))
## Fetch vector of dilutions
dilution <- filter(tab, target.dyeId == "FAM", sample.type == "std")$quantity

## Use plotCurves function from the chipPCR package to
## get an overview of the amplification curves
tmp <- as.data.frame(tmp)
plotCurves(tmp[,1], tmp[,-1])
par(mfrow = c(1,1))
## Use inder function from the chipPCR package to
## calculate the Cq (second derivative maximum, SDM)
SDMout <- sapply(2L:ncol(tmp), function(i) {
  SDM <- summary(inder(tmp[, 1], tmp[, i]), print = FALSE)[2]
})

## Use the effcalc function from the chipPCR package and
## plot the results for the calculation of the amplification
## efficiency analysis.
plot(effcalc(dilution, SDMout), CI = TRUE)

## End(Not run)
## Not run:
## EXAMPLE 3:
## internal dataset BioRad_qPCR_melt.rdml (in 'data' directory)
## generated by Bio-Rad CFX96. Contains qPCR and melting data.
## Import with custom name pattern.
PATH <- path.package("RDML")
filename <- paste(PATH, "/extdata/", "BioRad_qPCR_melt.rdml", sep = "")
cfx96 <- RDML$new(filename)
## Use plotCurves function from the chipPCR package to
## get an overview of the amplification curves
library(chipPCR)
## Extract all qPCR data
tab <- cfx96$AsTable()
cfx96.qPCR <- as.data.frame(cfx96$GetFDData(tab))
plotCurves(cfx96.qPCR[,1], cfx96.qPCR[,-1], type = "l")

## Extract all melting data
cfx96.melt <- cfx96$GetFDData(tab, dp.type = "mdp")
## Show some generated names for samples.
colnames(cfx96.melt)[2L:5]
## Select columns that contain
## samples with dye 'EvaGreen' and have type 'pos'
## using filtering by names.
cols <- cfx96$GetFDData(filter(tab, grepl("pos_EvaGreen$", fdata.name)),
                        dp.type = "mdp")
## Conduct melting curve analysis.
library(qpcR)
invisible(meltcurve(cols, fluos = 2:ncol(cols),

```



```
        temps = rep(1, ncol(cols) - 1)))  
  
## End(Not run)
```

RDML.AsDendrogram *Represents structure of RDML file as dendrogram*

Description

Plots and/or returns the structure of RDML file as [dendrogram](#) (tree-like structure.)

Arguments

plot.dendrogram
plots dendrogram if TRUE

Value

dendrogram object

Author(s)

Konstantin A. Blagodatskikh <k.blag@yandex.ru>, Stefan Roediger <stefan.roediger@b-tu.de>, Michal Burdukiewicz <michalburdukiewicz@gmail.com>

Examples

```
## Not run:  
PATH <- path.package("RDML")  
filename <- paste(PATH, "/extdata/", "BioRad_qPCR_melt.rdml", sep = "")  
cfx96 <- RDML$new(filename)  
#plot dendrogram  
cfx96$AsDendrogram()  
#assign dendrogram to the object  
dendr <- cfx96$AsDendrogram(plot.dendrogram = FALSE)  
  
## End(Not run)
```

RDML.AsTable	<i>Represents fields of RDML object as data.frame</i>
--------------	---

Description

Formats particular fields of RDML object as data.frames, filters or passes them to [RDML.GetFData](#) and [RDML.SetFData](#) functions.

Arguments

<code>.default</code>	list of default columns
<code>name.pattern</code>	expression to form <code>fdata.name</code> (see Examples)
<code>add.columns</code>	list of additional columns
<code>treat.null.as.na</code>	if value is NULL then convert it to NA. Helps to deal with incomplete records.
<code>...</code>	additional columns

Details

By default input this function forms data.frame with following columns:

exp.id experiment\$`id`
run.id run\$`id`
react.id react\$`id`
position react\$`position`
sample react\$`sample`
target data\$`target`
target.dyeId target[[data\$`id`]]\$`dyeId`
sample.type sample[[react\$`sample`]]\$`type`

You can overload default columns list by parameter `.default` but note that columns

`exp.id`, `run.id`, `react.id`, `target`

are necessary for usage `AsTable` output as input for `GetFData` and `SetFData`. Additional columns can be introduced by specifying them at input parameter `...` (see Examples). All default and additional columns accession expressions must be named.

Experiment, run, react and data to which belongs each fluorescence data vector can be accessed by `experiment`, `run`, `react`, `data` (see Examples).

Result table does not contain data from experiments with ids starting with `'?!'`

Author(s)

Konstantin A. Blagodatskikh <k.blag@yandex.ru>, Stefan Roediger <stefan.roediger@b-tu.de>, Michal Burdukiewicz <michalburdukiewicz@gmail.com>

Examples

```
## Not run:
## internal dataset stepone_std.rdml (in 'data' directory)
## generated by Applied Biosystems Step-One. Contains qPCR data.
library(chipPCR)
PATH <- path.package("RDML")
filename <- paste(PATH, "/extdata/", "stepone_std.rdml", sep = "")
stepone <- RDML$new(filename)
## Mark fluorescence data which Cq > 30 and add quantities to
## AsTable output.
## Names for fluorescence data will contain sample name and react
## positions
tab <- stepone$AsTable(
  name.pattern = paste(react$sample$id, react$position),
  add.columns = list(cq30 = if(data$cq >= 30) ">=30" else "<30",
    quantity = sample[[react$sample$id]]$quantity$value)
)
## Show cq30 and quantities
tab[, c("cq30", "quantity")]
## Get fluorescence values for 'std' type samples
## in format ready for ggplot function
library(dplyr)
fdata <- stepone$GetFData(
  filter(tab, sample.type == "std"),
  long.table = TRUE)
## Plot fdata with colour by cq30 and shape by quantity
library(ggplot2)
ggplot(fdata, aes(x = cyc, y = fluor,
  group = fdata.name,
  colour = cq30,
  shape = as.factor(quantity))) +
  geom_line() + geom_point()

## End(Not run)
```

RDML.GetFData

*Gets fluorescence data vectors from RDML object***Description**

Gets fluorescence data vectors from RDML object for specified method of experiment.

Arguments

request	Output from AsTable method(RDML.AsTable)
dp.type	Type of fluorescence data (i.e. 'adp' for qPCR or 'mdp' for melting)
long.table	Output table is ready for ggplot (See RDML.AsTable for example)

Value

matrix which contains selected fluorescence data and additional information from request if `long.table = TRUE`.

Author(s)

Konstantin A. Blagodatskikh <k.blag@yandex.ru>, Stefan Roediger <stefan.roediger@b-tu.de>, Michal Burdukiewicz <michalburdukiewicz@gmail.com>

Examples

```
## Not run:
## internal dataset BioRad_qPCR_melt.rdml (in 'data' directory)
## generated by Bio-Rad CFX96. Contains qPCR and melting data.
## Import without splitting by targets/types and with
## custom name pattern.
PATH <- path.package("RDML")
filename <- paste(PATH, "/extdata/", "BioRad_qPCR_melt.rdml", sep = "")
cfx96 <- RDML$new(filename)
## Select melting fluorescence data with sample.type 'unkn'.
library(dplyr)
tab <- cfx96$AsTable()
fdata <- cfx96$GetFData(filter(tab, sample.type == "unkn"),
                        dp.type = "adp")
## Show names for obtained fdata
colnames(fdata)

## End(Not run)
```

RDML.SetFData

Sets fluorescence data vectors to RDML object

Description

Sets fluorescence data vectors to RDML object for specified method of experiment.

Arguments

<code>data</code>	matrix containing in the first column data corresponding to all fluorescence values in the following columns. The name of the first column is the name of variable and names of other column are <code>fdata.names</code> (links to rows at description).
<code>description</code>	output from <code>AsTable</code> function that describes fluorescence data.
<code>fdata.type</code>	'adp' for qPCR, 'mdp' for melting data.

Examples

```

## Not run:
PATH <- path.package("RDML")
filename <- paste0(PATH, "/extdata/", "stepone_std.rdml")
cfx96 <- RDML$new(filename)
## Use plotCurves function from the chipPCR package to
## get an overview of the amplification curves
library(chipPCR)
## Extract all qPCR data
tab <- cfx96$AsTable()
tab2 <- tab
tab2$run.id <- "cpp"
cfx96.qPCR <- as.data.frame(cfx96$GetFData(tab))
cpp <- cbind(cyc = cfx96.qPCR[, 1],
  apply(cfx96.qPCR[, -1], 2,
    function(y) CPP(x = cfx96.qPCR[, 1], y = y)$y.norm))
cfx96$SetFData(cpp, tab2)
library(ggplot2)
library(gridExtra)
cfx96.gg <- cfx96$GetFData(tab, long.table = TRUE)
cpp.gg <- cfx96$GetFData(tab2,
  long.table = TRUE)
plot1 <- ggplot(cfx96.gg, aes(x = cyc, y = fluor,
  group=fdata.name)) +
  geom_line() +
  ggtitle("Raw data")
plot2 <- ggplot(cpp.gg, aes(x = cyc, y = fluor,
  group=fdata.name)) +
  geom_line() +
  ggtitle("CPP processed data")
grid.arrange(plot1, plot2, nrow=2)

## End(Not run)

```

rdmlBaseType

Base R6 class for RDML package.

Description

Most classes from RDML package inherit this class. It is designed for internal usage and should not be directly accessed.

Format

An [R6Class](#) generator object.

Initialization

`rdmlBaseType$new()`

Methods

`.asXMLnodes(node.name)` Represents object as XML nodes. Should not be called directly. `node.name`
– name of the root node for the generated XML tree.

`print(...)` prints object

Methods**Public methods:**

- `rdmlBaseType$.asXMLnodes()`
- `rdmlBaseType$copy()`
- `rdmlBaseType$print()`
- `rdmlBaseType$clone()`

Method `.asXMLnodes()`:

Usage:

`rdmlBaseType$.asXMLnodes(node.name)`

Method `copy()`:

Usage:

`rdmlBaseType$copy()`

Method `print()`:

Usage:

`rdmlBaseType$print(...)`

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

`rdmlBaseType$clone(deep = FALSE)`

Arguments:

`deep` Whether to make a deep clone.

rdmlEdit

RDML Editor Graphical User Interface

Description

Launches graphical user interface that can edit RDML metadata and show qPCR or melting curves.

Usage

`rdmlEdit()`

rdmlIdType	<i>rdmlIdType R6 class.</i>
------------	-----------------------------

Description

This element can be used to assign a publisher and id to the RDML file.
Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
rdmlIdType$new(publisher, serialNumber,  
MD5Hash = NULL)
```

Fields

publisher [checkString](#). RDML file publisher.

serialNumber [checkString](#). Serial number.

MD5Hash [checkString](#). An MD5Hash calculated over the complete file after removing all rdmlID-Types and all whitespaces between elements.

Super class

```
RDML::rdmlBaseType -> rdmlIdType
```

Methods

Public methods:

- [rdmlIdType\\$new\(\)](#)
- [rdmlIdType\\$clone\(\)](#)

Method new():

Usage:

```
rdmlIdType$new(publisher, serialNumber, MD5Hash = NULL)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
rdmlIdType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

reactIdType	<i>reactIdType R6 class.</i>
-------------	------------------------------

Description

Contains identifier for reactType. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
reactIdType$new(id)
```

@section Fields:

id [checkCount](#). Identifier.

Super classes

[RDML::rdmlBaseType](#) -> [RDML::idType](#) -> reactIdType

Methods

Public methods:

- [reactIdType\\$new\(\)](#)
- [reactIdType\\$clone\(\)](#)

Method new():

Usage:

```
reactIdType$new(id)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
reactIdType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

reactType	<i>reactType R6 class.</i>
-----------	----------------------------

Description

A reaction is an independent chemical reaction corresponding for example to a well in a 96 well plate, a capillary in a rotor, a through-hole on an array, etc. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Details

The ID of this reaction

Schemas :

- rotor : assign IDs according to the position of the sample on the rotor (1 for the 1st sample, 2 for the 2nd, ...)
- plate (96/384/1536 well) : the IDs are assigned in a row-first/column-second manner. For each row, the samples are numbered according to the increasing column number. At the end of a row, the numbering starts at the first column of the next row. An example for this type of plate can be found below :

	1	2	3	...
A	1	2	3	
B	13	14		
...				

or

	1	2	3	...
1	1	2	3	
2	13	14		
...				

- multi-array plate (BioTrove) : the IDs are assigned in a row-first/column-second manner, ignoring the organisation of sub-arrays. For each row, the samples are numbered according to the increasing column number. At the end of a row, the the next row. An example for this type of plate can be found below : todo...

Initialization

`reactType$new(id, sample, data = NULL, pcrFormat = pcrFormatType$new(8, 12, labelFormatType$new("123"))`

@section Fields:

`id` [reactIdType](#). See 'Details'.

sample [idReferencesType](#). SampleID - A reference to a sample.
 data list of [dataType](#).
 position Human readable form of the react id (i.e. '13' -> 'B1')..

Methods

`AsDataFrame(dp.type = "adp")` Represents amplification (dp.type = "adp") or melting (dp.type = "mdp") data points of all targets as one data.frame

`.recalcPosition(pcrformat)` Converts react id to the human readable form (i.e. '13' -> 'B1'). This converted value can be accessed by position field. pcrFormat is pcrFormatType. Currently, only 'ABC' and '123' are supported as labels. For '123' '123' the Position will look like 'r01c01', for 'ABC' '123' it will be 'A01' and for '123' 'ABC' it will be 01A. 'ABC' 'ABC' is not currently supported. Note that 'ABC' will result in loss of information if the experiment contains more than 26 rows!

Super class

`RDML::rdmlBaseType` -> reactType

Methods

Public methods:

- `reactType$new()`
- `reactType$GetFData()`
- `reactType$.recalcPosition()`
- `reactType$clone()`

Method new():

Usage:

```
reactType$new(
  id,
  sample,
  data = NULL,
  pcrFormat = pcrFormatType$new(8, 12, labelFormatType$new("ABC"),
    labelFormatType$new("123"))
)
```

Method GetFData():

Usage:

```
reactType$GetFData(dp.type = "adp", long.table = FALSE)
```

Method .recalcPosition():

Usage:

```
reactType$.recalcPosition(pcrFormat)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
reactType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

runType

runType R6 class.

Description

A run is a set of reactions performed in one "run", for example one plate, one rotor, one array, one chip. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
runType$new(id, description = NULL,
  documentation = NULL, experimenter = NULL, instrument = NULL,
  dataCollectionSoftware = NULL, backgroundDeterminationMethod = NULL,
  cqDetectionMethod = NULL, thermalCyclingConditions = NULL, pcrFormat,
  runDate = NULL, react = NULL)
```

Fields

id [idType](#).

description [checkString](#).

documentation list of [idReferencesType](#).

experimenter list of [idReferencesType](#).

instrument [checkString](#). Description of the instrument used to acquire the data.

dataCollectionSoftware [dataCollectionSoftwareType](#). Description of the software used to analyze/collect the data.

backgroundDeterminationMethod [checkString](#). Description of method used to determine the background.

cqDetectionMethod [cqDetectionMethodType](#). Description of method used to calculate the quantification cycle.

thermalCyclingConditions [idReferencesType](#). The program used to acquire the data.

pcrFormat [adpsType](#).

runDate [adpsType](#). Time stamp of data acquisition.

react list of [adpsType](#).

Methods

AsDataFrame(dp.type = "adp") Represents amplification (dp.type = "adp") or melting (dp.type = "mdp") data points as data.frame

Super class

RDML::rdmlBaseType -> runType

Methods**Public methods:**

- runType\$new()
- runType\$GetFDData()
- runType\$updateReactsPosition()
- runType\$clone()

Method new():

Usage:

```
runType$new(
  id,
  description = NULL,
  documentation = NULL,
  experimenter = NULL,
  instrument = NULL,
  dataCollectionSoftware = NULL,
  backgroundDeterminationMethod = NULL,
  cqDetectionMethod = NULL,
  thermalCyclingConditions = NULL,
  pcrFormat,
  runDate = NULL,
  react = NULL
)
```

Method GetFDData():

Usage:

```
runType$GetFDData(dp.type = "adp", long.table = FALSE)
```

Method UpdateReactsPosition():

Usage:

```
runType$updateReactsPosition()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
runType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

sampleType	<i>sampleType R6 class.</i>
------------	-----------------------------

Description

A sample is a template solution with defined concentration. Since dilutions of the same material differ in concentration, they are considered different samples. A technical replicate samples should contain the same name (reactions are performed on the same material), and biological replicates should contain different names (the template derived from the different biological replicates is divergent). Serial dilutions in a standard curve must have different names (preferably stating their dilution). Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
sampleType$new(id, description = NULL,
  documentation = NULL, xRef = NULL, annotation = NULL, type =
  sampleTypeType$new("unkn"), interRunCalibrator = FALSE, quantity = NULL,
  calibratorSample = FALSE, cdnaSynthesisMethod = NULL, templateQuantity =
  NULL)
```

@section Fields:

id [idType](#). Concentration of the template in nanogram per microliter in the final reaction mix.

description [checkString](#).

documentation list of [idReferencesType](#).

xRef list of [xRefType](#).

annotation list of [annotationType](#).

type [sampleTypeType](#).

interRunCalibrator [checkFlag](#). TRUE if this sample is used as inter run calibrator.

quantity [quantityType](#). Quantity - The reference quantity of this sample. It should be only used if the sample is part of a standard curve. The provided value will be used to quantify unknown samples in absolute quantification assays. Only the use of positive integers (like 1, 10, 100, 1000) and fractions (e.g. 1, 0.1, 0.01, 0.001) is acceptable. The use of exponents (1, 2, 3, 4 or -1, -2, -3, -4) is forbidden, because it will not be interpreted as 10E1, 10E2, 10E3, 10E4 or 10E-1, 10E-2, 10E-3, 10E-4.

calibratorSample [checkFlag](#). TRUE if this sample is used as calibrator sample.

cdnaSynthesisMethod [cdnaSynthesisMethodType](#).

templateQuantity [templateQuantityType](#).

Super class

[RDML::rdmlBaseType](#) -> sampleType

Methods**Public methods:**

- [sampleType\\$new\(\)](#)
- [sampleType\\$clone\(\)](#)

Method new():*Usage:*

```
sampleType$new(
  id,
  description = NULL,
  documentation = NULL,
  xRef = NULL,
  annotation = NULL,
  type = sampleTypeType$new("unkn"),
  interRunCalibrator = FALSE,
  quantity = NULL,
  calibratorSample = FALSE,
  cdnaSynthesisMethod = NULL,
  templateQuantity = NULL
)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
sampleType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

sampleTypeType

sampleTypeType R6 class.

Description

Can take values:

unkn unknown sample

ntc non template control

nac no amplification control

std standard sample

ntp no target present

nrt minusRT

pos positive control

opt optical calibrator sample

Format

An [R6Class](#) generator object.

Details

Inherits: [enumType](#).

Initialization

sampleTypeType\$new(value)

@section Fields:

value [checkString](#). Value.

Super classes

[RDML::rdmlBaseType](#) -> [RDML::enumType](#) -> sampleTypeType

Methods**Public methods:**

- [sampleTypeType\\$clone\(\)](#)

Method [clone\(\)](#): The objects of this class are cloneable with this method.

Usage:

```
sampleTypeType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

sequencesType

sequencesType R6 class.

Description

Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
sequencesType$new(forwardPrimer = NULL,  
reversePrimer = NULL, probe1 = NULL, probe2 = NULL, amplicon = NULL)
```

@section Fields:

forwardPrimer [oligoType](#).

reversePrimer [oligoType](#).

probe1 [oligoType](#).

probe2 [oligoType](#).

amplicon [oligoType](#).

Super class

```
RDML::rdmlBaseType -> sequencesType
```

Methods**Public methods:**

- [sequencesType\\$new\(\)](#)
- [sequencesType\\$clone\(\)](#)

Method new():

Usage:

```
sequencesType$new(  
  forwardPrimer = NULL,  
  reversePrimer = NULL,  
  probe1 = NULL,  
  probe2 = NULL,  
  amplicon = NULL  
)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
sequencesType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

SetFData	RDML\$SetFData() <i>wrapper</i>
----------	---------------------------------

Description

Read more at [RDML.SetFData](#)

Usage

```
SetFData(obj, ...)
```

Arguments

obj	RDML object.
...	SetFData params.

stepType	<i>stepType R6 class.</i>
----------	---------------------------

Description

Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
stepType$new(nr, description = NULL,
  temperature = NULL, gradient = NULL, loop = NULL, pause = NULL, lidOpen =
  NULL)
```

Fields

nr [checkCount](#). The incremental number of the step. First step should have value 1. The increment between steps should be constant and equivalent to 1.

description [checkString](#).

temperature [temperatureType](#).

gradient [gradientType](#).

loop [loopType](#).

pause [pauseType](#).

lidOpen [lidOpenType](#).

Super class

`RDML::rdmlBaseType` -> `stepType`

Methods**Public methods:**

- `stepType$new()`
- `stepType$clone()`

Method new():

Usage:

```
stepType$new(
  nr,
  description = NULL,
  temperature = NULL,
  gradient = NULL,
  loop = NULL,
  pause = NULL,
  lidOpen = NULL
)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
stepType$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

targetType

targetType R6 class.

Description

A target is a PCR reaction with defined set of primers. PCR reactions for the same gene with distinct primer sequences are considered different targets. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
targetType$new(id, description = NULL,
  documentation = NULL, xRef = NULL, type, amplificationEfficiencyMethod =
  NULL, amplificationEfficiency = NULL, amplificationEfficiencySE = NULL,
  detectionLimit = NULL, dyeId, sequences = NULL, commercialAssay = NULL)
```

Fields

id [idType](#).
description [checkString](#).
documentation list of [idReferencesType](#).
xRef list of [xRefType](#).
type [targetTypeType](#).
amplificationEfficiencyMethod [checkString](#).
amplificationEfficiency [checkNumber](#).
amplificationEfficiencySE [checkNumber](#).
detectionLimit [checkNumber](#).
dyeId [idReferencesType](#).
sequences [sequencesType](#).
commercialAssay [commercialAssayType](#).

Super class

[RDML::rdmlBaseType](#) -> targetType

Methods**Public methods:**

- [targetType\\$new\(\)](#)
- [targetType\\$clone\(\)](#)

Method new():

Usage:

```
targetType$new(  
  id,  
  description = NULL,  
  documentation = NULL,  
  xRef = NULL,  
  type,  
  amplificationEfficiencyMethod = NULL,  
  amplificationEfficiency = NULL,  
  amplificationEfficiencySE = NULL,  
  detectionLimit = NULL,  
  dyeId,  
  sequences = NULL,  
  commercialAssay = NULL  
)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
targetType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

targetTypeType *targetTypeType R6 class.*

Description

Can take values:

ref reference target

toi target of interest

Inherits: [enumType](#).

Format

An [R6Class](#) generator object.

Initialization

targetTypeType\$new(value)

@section Fields:

value [checkString](#).

Super classes

[RDML::rdmlBaseType](#) -> [RDML::enumType](#) -> targetTypeType

Methods

Public methods:

- [targetTypeType\\$clone\(\)](#)

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
targetTypeType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

temperatureType *temperatureType R6 class.*

Description

This step keeps a constant temperature on the heat block. Inherits: [baseTemperatureType](#).

Format

An [R6Class](#) generator object.

Initialization

```
temperatureType$new(temperature, ...)
```

Fields

temperature [checkNumber](#). The temperature of the step in degrees Celsius.
... Params of parent class [baseTemperatureType](#).

Super classes

```
RDML::rdmlBaseType -> RDML::baseTemperatureType -> temperatureType
```

Methods

Public methods:

- [temperatureType\\$new\(\)](#)
- [temperatureType\\$clone\(\)](#)

Method new():

Usage:

```
temperatureType$new(temperature, ...)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
temperatureType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

templateQuantityType *templateQuantityType R6 class.*

Description

Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
templateQuantityType$new(conc, nucleotide)
```

@section Fields:

conc [checkNumber](#). Concentration of the template in nanogram per microliter in the final reaction mix.

nucleotide [nucleotideType](#).

Super class

```
RDML::rdmlBaseType -> templateQuantityType
```

Methods

Public methods:

- [templateQuantityType\\$new\(\)](#)
- [templateQuantityType\\$clone\(\)](#)

Method new():

Usage:

```
templateQuantityType$new(conc, nucleotide)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
templateQuantityType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

thermalCyclingConditionsType
thermalCyclingConditionsType R6 class.

Description

A cycling program for PCR or to amplify cDNA. Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
thermalCyclingConditionsType$new(id,  
  description = NULL, documentation = NULL, lidTemperature = NULL,  
  experimenter = NULL, step)
```

Fields

id [idType](#).
description [checkString](#).
documentation list of [idReferencesType](#).
lidTemperature [checkNumber](#). The temperature in degrees Celsius of the lid during cycling.
experimenter list of [idReferencesType](#). Reference to the person who made or uses this protocol.
step list of [stepType](#). The steps a protocol runs through to amplify DNA.

Super class

```
RDML::rdmlBaseType -> thermalCyclingConditionsType
```

Methods

Public methods:

- [thermalCyclingConditionsType\\$new\(\)](#)
- [thermalCyclingConditionsType\\$clone\(\)](#)

Method new():

Usage:

```
thermalCyclingConditionsType$new(  
  id,  
  description = NULL,  
  documentation = NULL,  
  lidTemperature = NULL,  
  experimenter = NULL,  
  step  
)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
thermalCyclingConditionsType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

xRefType

xRefType R6 class.

Description

Inherits: [rdmlBaseType](#).

Format

An [R6Class](#) generator object.

Initialization

```
xRefType$new(name = NULL, id = NULL)
```

@section Fields:

name [checkString](#). Reference to an external database, for example "GenBank".

id [checkString](#). The ID of the entry within the external database, for example "AJ832138".

Super class

```
RDML::rdmlBaseType -> xRefType
```

Methods

Public methods:

- [xRefType\\$new\(\)](#)
- [xRefType\\$clone\(\)](#)

Method new():

Usage:

```
xRefType$new(name = NULL, id = NULL)
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
xRefType$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

[.GetFData *Extract data points from RDML object*

Description

Extract data points from RDML object as.data.frame.

Usage

```
## S3 method for class 'RDML'  
x[i, j, dp.type = "adp"]
```

Arguments

x	RDML object.
i, j	indices.
dp.type	Type of fluorescence data (i.e. 'adp' for qPCR or 'mdp' for melting).

Index

- * **Bio-Rad**
 - RDML, 36
- * **CFX96**
 - RDML, 36
- * **IO**
 - RDML, 36
- * **LightCycler**
 - RDML, 36
- * **RDML**
 - RDML, 36
- * **StepOne**
 - RDML, 36
- * **file**
 - RDML, 36
- * **hplot**
 - rdmIEdit, 46
- * **manip**
 - [.GetFData, 65
 - as.character.idType, 6
 - as.character.reactIdType, 6
 - RDML.AsDendrogram, 41
 - RDML.AsTable, 42
 - RDML.GetFData, 43
- * **qPCR**
 - RDML, 36
 - [.GetFData, 65
 - [.RDML ([.GetFData), 65
- adpsType, 3, 13, 51
- annotationType, 5, 53
- as.character.idType, 6
- as.character.reactIdType, 6
- AsDendrogram, 7
- assertCount, 25
- assertMatrix, 3, 26
- AsTable, 7
- baseTemperatureType, 8, 20, 61
- cdnaSynthesisMethodType, 9, 53
- checkCount, 8, 33, 48, 57
- checkFlag, 9, 53
- checkNumber, 8, 13, 20, 31, 34, 59, 61–63
- checkString, 5, 9–13, 15, 16, 18, 19, 21–23, 27, 30, 34, 36, 47, 51, 53, 55, 57, 59, 60, 63, 64
- commercialAssayType, 10, 59
- cqDetectionMethodType, 11, 51
- dataCollectionSoftwareType, 12, 51
- dataType, 13, 50
- dendrogram, 41
- documentationType, 14
- dyeType, 15
- enumType, 11, 16, 23, 27, 30, 34, 35, 55, 60
- experimenterType, 17
- experimentType, 19
- GetFData, 20
- gradientType, 20, 57
- idReferencesType, 9, 13, 19, 21, 50, 51, 53, 59, 63
- idType, 15, 18, 19, 21, 22, 51, 53, 59, 63
- labelFormatType, 23, 33
- lidOpenType, 24, 57
- loopType, 25, 57
- mdpsType, 13, 26
- measureType, 8, 27
- MergeRDMLs, 28, 37
- new, 28
- nucleotideType, 29, 62
- oligoType, 30, 56
- pauseType, 31, 57
- pcrFormatType, 23, 32

primingMethodType, 9, 33

quantityType, 34, 53

quantityUnitType, 34, 35

R6Class, 3, 5, 8–17, 19–27, 30–32, 34–36, 45, 47–49, 51, 53, 55, 57, 58, 60–64

RDML, 36

RDML.AsDendrogram, 7, 37, 41

RDML.AsTable, 7, 37, 42, 43

RDML.GetFData, 20, 37, 42, 43

RDML.new, 36, 37

RDML.new (new), 28

RDML.SetFData, 37, 44, 57

RDML::baseTemperatureType, 21, 61

RDML::enumType, 11, 23, 27, 30, 34, 36, 55, 60

RDML::idType, 21, 48

RDML::rdmlBaseType, 3, 5, 8–12, 14–16, 18, 19, 21–27, 30, 31, 33–37, 47, 48, 50, 52, 53, 55, 56, 58–64

rdmlBaseType, 3, 5, 8–10, 12–17, 19, 22, 24–26, 30–32, 34, 45, 47–49, 51, 53, 55, 57, 58, 62–64

rdmlEdit, 46

rdmlIdType, 47

reactIdType, 48, 49

reactType, 49

runType, 19, 51

sampleType, 53

sampleTypeType, 53, 54

sequencesType, 55, 59

SetFData, 57

stepType, 57, 63

targetType, 58

targetTypeType, 59, 60

temperatureType, 57, 61

templateQuantityType, 53, 62

thermalCyclingConditionsType, 63

xRefType, 53, 59, 64