Package 'Structstrings'

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Title Implementation of the dot bracket annotations with Biostrings

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Description The Structstrings package implements the widely used dot bracket annotation for storing base pairing information in structured RNA. Structstrings uses the infrastructure provided by the Biostrings package and derives the DotBracketString and related classes from the BString class. From these, base pair tables can be produced for in depth analysis. In addition, the loop indices of the base pairs can be retrieved as well. For better efficiency, information conversion is implemented in C, inspired to a large extend by the ViennaRNA package.

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`Structstrings-package` *Structstrings: Implementation of the dot bracket annotations with Biostrings*

Description

The Structstrings package implements the widely used dot bracket annotation for storing base pairing information in structured RNA. Structstrings uses the infrastructure provided by the Biostrings package and derives the DotBracketString and related classes from the BString class. From these, base pair tables can be produced for in depth analysis. In addition, the loop indices of the base pairs can be retrieved as well. For better efficiency, information conversion is implemented in C, inspired to a large extend by the ViennaRNA package.

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See Also

Useful links:

- https://github.com/FelixErnst/Structstrings
- Report bugs at https://github.com/FelixErnst/Structstrings/issues

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`convertAnnotation` *Convert between dot bracket annotations*

Description

`convertAnnotation` converts a type of dot bracket annotation into another. This only works if the original bracket type is present and the target bracket type is not.

Usage

```
convertAnnotation(x, from, to)

## S4 method for signature 'DotBracketString'
convertAnnotation(x, from, to)

## S4 method for signature 'DotBracketStringSet'
convertAnnotation(x, from, to)

## S4 method for signature 'DotBracketStringSetList'
convertAnnotation(x, from, to)
```

Arguments

`x`	a `DotBracketString`, `DotBracketStringSet` or `DotBracketStringSetList`
`from`	which annotation type should be converted? Must be one of the following values: `1L = '()'`, `2L = '<>'`, `3L = '[]'`, `4L = '{}'` and must be present in the input.
`to`	Into which annotation type should the selected one be converted? Must be one of the following values: `1L = '()'`, `2L = '<>'`, `3L = '[]'`, `4L = '{}'`. Must not be present in the input.

Value

The modified input object, a `DotBracketString*` object.

Examples

```
str <- "((.))..[[..]]...{{..}}......."
dbs <- DotBracketString(str)
convertAnnotation(dbs, 1L, 2L)
```

DotBracketDataFrame *DataFrame for storing base pairing information*

Description

The DotBracketDataFrame and DotBracketDFrame object is derived from the DataFrame and DFrame classes. DotBracketDataFrame implents the concept and can be used to implement other backends than the in-memory one as done by DotBracketDFrame.

The DotBracketDataFrameList is implemented analogous, which is also available as CompressedSplitDotBracketDa
Since the names are quite long, the following short cut functions are available for object creation: DBDF, DBDFL and SDBDFL.

The DotBracketDataFrame can only contain 5 columns, which are named pos, forward, reverse, character and base. The last two columns are optional. The type of the first three has to be integer, whereas the fourth is a character and fifth is a XStringSet column.

Upon creation and modification, the validity of the contained base pairing information is checked. If the information is not correct, an error is thrown.

Usage

```
DotBracketDataFrame(..., row.names = NULL)

DBDF(...)

DotBracketDataFrameList(...)

DBDFL(...)

SplitDotBracketDataFrameList(..., compress = TRUE, cbindArgs = FALSE)

SDBDFL(..., compress = TRUE, cbindArgs = FALSE)
```

Arguments

...	for DotBracketDataFrame the input vectors and for DotBracketDataFrameList the DataFrame or the DotBracketDataFrame objects.
row.names	See DataFrame
compress	If compress = TRUE, returns a CompressedSplitDotBracketDataFrameList else returns a SimpleSplitDotBracketDataFrameList.
cbindArgs	If cbindArgs = FALSE, the ... arguments are coerced to DotBracketDataFrame objects and concatenated to form the result. If cbindArgs = TRUE, the arguments are combined as columns. The arguments must then be the same length, with each element of an argument mapping to an element in the result.

Value

a DotBracketDataFrame* object.

Examples

```
# Manual creation
df <- DataFrame(pos = c(1,2,3,4,5,6),
                forward = c(6,5,0,0,2,1),
                reverse = c(1,2,0,0,5,6))
# Either works
dbdf <- as(df,"DotBracketDataFrame")
dbdf <- DotBracketDataFrame(df)
# With multiple input DataFrames a SplitDotBracketDataFrameList is returned
dbdfl <- DotBracketDataFrame(df,df,df,df)

# Creation from a DotBracketString object is probably more common
data("dbs", package = "Structstrings")
dbdfl <- getBasePairing(dbs)
# Elements are returned as DotBracketDataFrames
dbdfl[[1]]
```

DotBracketString *The DotBracketString, DotBracketStringSet and DotBracketStringSetList classes*

Description

The DotBracketString extends the BString class. The DotBracketStringSet and DotBracketStringSetList classes are implemented accordingly.

The alphabet consists of the letters (,), ., <, >, [,], { and }, which describes base pairing between positions. The . letter describes an unpaired position. The number of opening and closing letters need to be equal within a DotBracketString to be a valid dot bracket annotation. This is checked upon creation and modificiation of the object.

The objects can also be created using the shorter function names DB, DBS and DBSL.

Currently, there is no distinction in base pairing strength between the different bracket types.

Usage

```
DotBracketString(x = "", start = 1, nchar = NA)

DB(x = character(), start = 1, nchar = NA)

DotBracketStringSet(x = character())

DBS(x = character())

DotBracketStringSetList(..., use.names = TRUE)

DBSL(..., use.names = TRUE)

## S4 method for signature 'DotBracketString'
alphabet(x)

## S4 method for signature 'DotBracketString'
encoding(x)
```

Arguments

x	DotBracketString,DotBracketStringSet: the input, which is tried to be convert into a DotBracketString*.
start	DotBracketString: starting position for creating the object from the character input.
nchar	DotBracketString: number of letters are read from the input character
...	DotBracketStringSetList: the input, which converted into a list. Each element is tried to be converted into a DotBracketStringSet.
use.names	DotBracketStringSetList: Should names of the input be preserved.

Value

a DotBracketString* object.

Examples

```
str <- "((.))..[[..]]...{{..}}..<<..>>"
db <- DotBracketString(str)
dbs <- DotBracketStringSet(c("structure1" = str, "structure2" = str))
dbsl <- DotBracketStringSetList(list(first = dbs, second = dbs))
```

DotBracketStringSet-io

Reading and writing DotBracketStringSet objects

Description

readDotBracketStringSet and writeDotBracketStringSet are functions to read and write dot bracket strings from/to file. Since the <> is in conflict with the fasta format, saving to fastq file is sometimes the only option. Saving a string with a <> bracket type to a fasta file will throw an error.

The functions use the underlying Biostrings infrastructure and share most of its parameters. For a more detailed look have a look here.

Usage

```
readDotBracketStringSet(
  filepath,
  format = "fasta",
  nrec = -1L,
  skip = 0L,
  seek.first.rec = FALSE,
  use.names = TRUE,
  with.qualities = FALSE
)

writeDotBracketStringSet(
  x,
  filepath,
  append = FALSE,
```

```
  compress = FALSE,
  format = "fasta",
  ...
)

saveDotBracketStringSet(
  x,
  objname,
  dirpath = ".",
  save.dups = FALSE,
  verbose = TRUE
)
```

Arguments

filepath	The file name, when writing, or file name(s) when reading.
format	"fasta" or "fastq"
nrec	Single integer. The maximum of number of records to read in. Negative values are ignored.
skip	Single non-negative integer. The number of records of the data file(s) to skip before beginning to read in records.
seek.first.rec, with.qualities, compress, ..., use.names, objname, dirpath, save.dups, verbose	Have a look here.
x	A DotBracketStringSet object
append	TRUE or FALSE. If TRUE output will be appended to file. Otherwise, it will overwrite the contents of file.

Value

readDotBracketStringSet returns a DotBracketStringSet object, writeDotBracketStringSet returns NULL invisibly.

Examples

```
data("dbs", package = "Structstrings")
file <- tempfile()
# works both since a DotBracketStringSet is a BStringSet
writeXStringSet(dbs,file)
writeDotBracketStringSet(dbs,file)
# to return immediatly a DotBracketStringSet us readDotBracketStringSet()
dbs2 <- readDotBracketStringSet(file)
```

---

getBasePairing *Accessing Dot Bracket annotation*

Description

getBasePairing converts a dot bracket annotation from a DotBracketString into a base pair table as DotBracketDataFrame. Base pairing is indicated by corresponding numbers in the forward and reverse columns.

getDotBracket converts the dot bracket annotation from a DotBracketDataFrame into a DotBracketString. If the character colums is populated, the information from this column will be used. If this is not desired set force = TRUE. However , beaware that this will result in a dot bracket annotation, which does not necessarilly matches the original dot bracket string it may have been created from. It is rather the dot bracket string with the lowest number of different loops and it will use the different dot bracket annotations one after another. Example: "(((«<»>)))" will be returned as ((((((.)))))). (((<«)))>» will be returned as (((<«)))>», ((([[[)))]]] will be eturned as (((<«)))>».

getLoopIndices converts the dot bracket annotation from a DotBracketString or DotBracketDataFrame into a LoopIndexList.

Usage

```
getBasePairing(x, compress = TRUE, return.sequence = FALSE)

getDotBracket(x, force = FALSE)

getLoopIndices(x, bracket.type, warn.type.drops = TRUE)

## S4 method for signature 'DotBracketString'
getBasePairing(x)

## S4 method for signature 'DotBracketStringSet'
getBasePairing(x, compress = TRUE)

## S4 method for signature 'DotBracketDataFrame'
getDotBracket(x, force = FALSE)

## S4 method for signature 'DotBracketDataFrameList'
getDotBracket(x, force = FALSE)

## S4 method for signature 'SimpleSplitDotBracketDataFrameList'
getDotBracket(x, force = FALSE)

## S4 method for signature 'CompressedSplitDotBracketDataFrameList'
getDotBracket(x, force = FALSE)

## S4 method for signature 'DotBracketString'
getLoopIndices(x, bracket.type, warn.type.drops = TRUE)

## S4 method for signature 'DotBracketStringSet'
getLoopIndices(x, bracket.type, warn.type.drops = TRUE)

## S4 method for signature 'DotBracketDataFrame'
getLoopIndices(x, bracket.type, warn.type.drops = TRUE)

## S4 method for signature 'DotBracketDataFrameList'
getLoopIndices(x, bracket.type, warn.type.drops = TRUE)
```

```
## S4 method for signature 'SimpleSplitDotBracketDataFrameList'
getLoopIndices(x, bracket.type, warn.type.drops = TRUE)

## S4 method for signature 'CompressedSplitDotBracketDataFrameList'
getLoopIndices(x, bracket.type, warn.type.drops = TRUE)
```

Arguments

x	a DotBracketString or DotBracketStringSet object
compress	getBasePairing: whether to return a CompressedSplitDotBracketDataFrameList or a SimpleSplitDotBracketDataFrameList
return.sequence	if the input is a StructuredXStringSet: TRUE(default) or FALSE: Whether the sequence should be returned in the base column.
force	getDotBracket: Should the dot bracket string be generated from the base pairing, if the character column is present?
bracket.type	getLoopIndices: Which dot bracket annotation type should be converted into loop indices? Only usable, if more than one is present. (1L = '()', 2L = '<>', 3L = '[]', 4L = '{}')
warn.type.drops	getLoopIndices: TRUE(default) or FALSE: Warn if more than one dot bracket annotation type is present in the input?

Value

getBasePairing: The result is a DotBracketDataFrame with following columns: pos, forward, reverse, character (and optionally the base column). If a position is unpaired, forward and reverse will be 0, otherwise it will match the base paired positions.

getLoopIndices: returns a LoopIndexList.

Examples

```
data("dbs", package = "Structstrings")
# conversion
dbdf <- getBasePairing(dbs)
# ... and the round trip
dbs <- getDotBracket(dbdf)

# loop indices per bracket type
loopids <- getLoopIndices(dbs)
# choose the bracket type manually, if necessary
loopids <- getLoopIndices(dbs, bracket.type = 1L)
# do not show warning if mulitple bracket types are present
loopids <- getLoopIndices(dbs, bracket.type = 1L, warn.type.drops = FALSE)
```

LoopIndexList *LoopIndexList: base pairing information as a list of integer values*

Description

With loop indeces base pairing information can be represented by giving each base pair a number and increasing/decreasing it with each opened/closed base pair. This information can be used for further analysis of the represented structure.

Usage

```
LoopIndexList(...)
```

Arguments

...	the integer input vectors.

Value

a LoopIndexList object.

Examples

```
# if the object is create manually make sure it is a valid structure
# information. Otherwise an error is thrown.
lil <- LoopIndexList(list(c(1L,2L,3L,3L,3L,2L,1L,0L,5L,6L,6L,5L),
                          c(1L,2L,2L,2L,2L,2L,1L,0L,5L,6L,6L,5L)))
```

Structstrings *Structstrings: implementation of the dot bracket annotations with Biostrings*

Description

The Structstrings package implements the widely used to bracket annotation for storing base pairing information in structured RNA. For example it is used in the ViennaRNA package (Lorenz et al. 2011), the tRNAscan-SE software (Lowe et al. 1997) and the tRNAdb (Jühling et al. 2009).

Structstrings uses the infrastructure provided by the Biostrings package and derives the class DotBracketString and such from the equivalent BString class. From these base pair table can be produced for in depth analysis. For this purpose the DotBracketDataFrame class is derived from the DataFrame class. In addition the loop IDs of the base pairs can be retrieved as a LoopIndexList, a derivate if the IntegerList. Generally, it checks automatically for the validity of the dot bracket annotation.

The conversion of the DotBracketString to the base pair table and the loop indices is implemented in C for efficiency. The C implementation to a large extent inspired by the ViennaRNA package.

This package was developed as a requirement for the tRNA package. However, other projects might benefit as well, so it was split of and improved upon.

Manual

Please refer to the Structstrings vignette for an example how to work and use the package: Structstrings.

Author(s)

Felix G M Ernst [aut,cre]

References

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Jühling, Frank; Mörl, Mario; Hartmann, Roland K.; Sprinzl, Mathias; Stadler, Peter F.; Pütz, Joern (2009): "TRNAdb 2009: Compilation of tRNA Sequences and tRNA Genes." Nucleic Acids Research 37 (suppl_1): D159–D162. doi:10.1093/nar/gkn772.

`Structstrings-data` *Structstrings example data*

Description

Example data for using the Structstrings package

Usage

```
data(dbs)

data(nseq)
```

Format

object of class `DotBracketStringSet` and `DNAStringSet`

An object of class `DNAStringSet` of length 299.

Source

sequence and dot bracket annotation of tRNAscan-SE output for *S. cerevisiae* imported using `tRNAscanImport`. The example file is part of the `tRNAscanImport` package.

Structstrings-internals
Structstrings internals

Description

Analog to Biostrings there are a few objects, which should only be used internally, but may be of use to other package developers. Otherwise take care.

Usage

```
DOTBRACKET_CHAR_VALUES

DOTBRACKET_ALPHABET

STRUCTURE_NEUTRAL_CHR

STRUCTURE_OPEN_CHR

STRUCTURE_CLOSE_CHR

## S4 replacement method for signature 'DotBracketDataFrame'
x[i, j, ...] <- value

## S4 replacement method for signature 'CompressedSplitDotBracketDataFrameList'
colnames(x) <- value

## S4 method for signature 'DotBracketString'
seqtype(x)

## S4 method for signature 'DotBracketString'
subseq(x, start = NA, end = NA, width = NA)

## S4 replacement method for signature 'DotBracketString'
subseq(x, start = NA, end = NA, width = NA) <- value

## S4 replacement method for signature 'DotBracketStringSet'
subseq(x, start = NA, end = NA, width = NA) <- value
```

Arguments

seqtype, x, start, end, width, value, i, j, ...
: used internally

Format

a integer vector of length 9 containing the integer values of the dotbracket alphabet

a character vector of length 9 containing the single characters of the dotbracket alphabet

a character vector of length 1 containing the character for unpaired positions

a character vector of length 4 containing the opening character of the dotbracket alphabet

a character vector of length 4 containing the closing character of the dotbracket alphabet

Examples

```
DOTBRACKET_CHAR_VALUES
DOTBRACKET_ALPHABET
STRUCTURE_NEUTRAL_CHR
STRUCTURE_OPEN_CHR
STRUCTURE_CLOSE_CHR

# the replace method for a DotBracketDataFrame had to be reimplemented
# because of the requirement of columns for a DotBracketDataFrameList and
# DotBracketDataFrame
data("dbs", package = "Structstrings")
dbdfl <- getBasePairing(dbs)
# Elements are returned as DotBracketDataFrames
dbdf <- dbdfl[[1]]
dbdfl[[1]] <- dbdf
dbdfl[1] <- dbdfl[1]
```

StructuredXStringSet *StructuredRNAStringSet for storing DotBracketAnnotation alongside nucleotide sequences*

Description

The StructuredXStringSet class can be used to store structure information alongside RNA sequences. The class behaves like the QualityScaledXStringSet classes.

Please note, that this does not check for validity regarding base pairing capabilities.

Usage

```
StructuredRNAStringSet(x, structure)

dotbracket(x)

dotbracket(x) <- value

## S4 method for signature 'StructuredXStringSet'
dotbracket(x)

## S4 replacement method for signature 'StructuredXStringSet'
dotbracket(x) <- value

readStructuredRNAStringSet(
  filepath,
  nrec = -1L,
  skip = 0L,
  seek.first.rec = FALSE,
  use.names = TRUE
)

writeStructuredXStringSet(x, filepath, append = FALSE, compress = FALSE, ...)
```

```
## S4 method for signature 'StructuredXStringSet'
getBasePairing(x, compress = TRUE, return.sequence = FALSE)

## S4 method for signature 'StructuredXStringSet'
getLoopIndices(x, bracket.type, warn.type.drops = TRUE)
```

Arguments

x	For the Structured*StringSet constructors: Either a character vector, or an RNAString, RNAStringSet object. For writeStructuredXStringSet: A StructuredRNAStringSe derivative.
structure, value	A DotBracketStringSet
use.names, type, filepath, nrec, skip, seek.first.rec, append, ...	See DotBracketStringSet-io
compress	See getBasePairing or DotBracketStringSet-io
return.sequence	TRUE(default) or FALSE: Whether the sequence should be returned in the base column.
bracket.type	getLoopIndices: Which dot bracket annotation type should be converted into loop indices? Only usable, if more than one is present. (1L = '()', 2L = '<>', 3L = '[]', 4L = '{}')
warn.type.drops	See getLoopIndices

Details

the dotbracket function allows access to the included DotBracketStringSet.

Value

a StructuredRNAStringSet object.

Examples

```
str <- DotBracketStringSet("(())")
seq <- RNAStringSet("AGCU")
sdbs <- StructuredRNAStringSet(seq,str)
```

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