

# Package ‘XNAString’

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**Title** Efficient Manipulation of Modified Oligonucleotide Sequences

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**Description** The XNAString package allows for description of base sequences and associated chemical modifications in a single object. XNAString is able to capture single stranded, as well as double stranded molecules. Chemical modifications are represented as independent strings associated with different features of the molecules (base sequence, sugar sequence, backbone sequence, modifications) and can be read or written to a HELM notation. It also enables secondary structure prediction using RNAfold from ViennaRNA. XNAString is designed to be efficient representation of nucleic-acid based therapeutics, therefore it stores information about target sequences and provides interface for matching and alignment functions from Biostrings and pwalgn packages.

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'XNAString2Helm.R' 'XNAStringFromHelm.R' 'alphabetFrequency.R'  
'data.R' 'dictFromMimir.R' 'dinucleotideFrequency.R'  
'globals.R' 'helm2String.R' 'matchPDict.R' 'matchPattern.R'  
'pairwiseAlignment.R' 'predictDuplexStructure.R'  
'predictMfeStructure.R' 'reverseComplement.R'

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alphabetFrequency	<i>XNAAlphabetFrequency returns letters frequency for a given object in base, sugar or backbone slot</i>
-------------------	--

---

### Description

XNAAlphabetFrequency returns letters frequency for a given object in base, sugar or backbone slot

XNAAlphabetFrequency method returns alphabet frequency for a given object. It works for 3 slots: base, sugar and backbone. If matrix\_nbr equals 1, alphabet frequency for the first elements in the slot is returned. Letters can be given as argument, otherwise unique letters in object's dictionary are in use.

### Usage

```
XNAAlphabetFrequencyFun(
  obj,
  slot,
  letters = NA,
  matrix_nbr = 1,
  as.prob = FALSE,
  base_only = FALSE
```

```

)

XNAAlphabetFrequency(
  obj,
  slot,
  letters = NA,
  matrix_nbr = 1,
  as.prob = FALSE,
  base_only = FALSE,
  ...
)

## S4 method for signature 'XNAString'
XNAAlphabetFrequency(
  obj,
  slot,
  letters = NA,
  matrix_nbr = 1,
  as.prob = FALSE,
  base_only = FALSE
)

## S4 method for signature 'XNAStringSet'
XNAAlphabetFrequency(
  obj,
  slot,
  letters = NA,
  matrix_nbr = 1,
  as.prob = FALSE,
  base_only = FALSE
)

```

### Arguments

obj	XNAString or XNAStringSet class
slot	string (slot name: base, sugar or backbone)
letters	character (or character vector)
matrix_nbr	numeric (1 or 2, if 1 - first slot's element is use, if 2 - 2nd element in slot)
as.prob	logical - if TRUE frequency returned as probability of occurrence
base_only	logical - if TRUE, frequency checked for 'A', 'C', 'G', 'T', other
...	optional arguments to generic function to support additional methods

### Value

matrix (frequency matrix for a given slot)

**Examples**

```

xnastring_obj <- XNAString(
  name = "b",
  base = c("AACCC", "GGEE"),
  sugar = c("FFOO", "OODD")
)
XNAAlphabetFrequency(obj = xnastring_obj,
  slot = "base")
XNAAlphabetFrequency(obj = xnastring_obj,
  slot = "base",
  as.prob = TRUE)
XNAAlphabetFrequency(obj = xnastring_obj,
  slot = "base",
  base_only = TRUE)
XNAAlphabetFrequency(obj = xnastring_obj,
  slot = "base",
  letters = c("A", "C"))
XNAAlphabetFrequency(obj = xnastring_obj,
  slot = "base",
  matrix_nbr = 2)

xnastring_obj_2 <- XNAString(
  base = c("ATCG"),
  sugar = c("FOOD"),
  backbone = c("SBB")
)
XNAStringSet_obj <- XNAStringSet(objects = list(
  xnastring_obj,
  xnastring_obj_2
))
XNAAlphabetFrequency(XNAStringSet_obj, "sugar")

```

backbone

*Backbone setter/getter method***Description**

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

**Usage**

```

backbone(x, ...)

## S4 method for signature 'XNAString'
backbone(x)

## S4 method for signature 'XNAStringSet'
backbone(x, i = 1)

```

```
backbone(x, ...) <- value

## S4 replacement method for signature 'XNAString'
backbone(x) <- value

## S4 replacement method for signature 'XNAStringSet'
backbone(x, i = 1) <- value
```

### Arguments

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
i	numeric - possibilities: 1 or 2. If 1 - 1st slots elements printed out, 2nd otherwise. In case the second element is not in the object, empty char created. This parameter is only available for XNAStringSet objects.
value	character vector applied only for setter method

### Details

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. `name<-` method overwrites existing name slot

### Value

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

### Examples

```
my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj <- XNAString(
  name = "b",
  base = "GGE",
  sugar = "FFO",
  dictionary = my_dic
)
backbone(obj)
```

---

base	<i>Base setter/getter method</i>
------	----------------------------------

---

### Description

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

### Usage

```
base(x, ...)  
  
## S4 method for signature 'XNAString'  
base(x)  
  
## S4 method for signature 'XNAStringSet'  
base(x, i = 1)  
  
base(x, ...) <- value  
  
## S4 replacement method for signature 'XNAString'  
base(x) <- value  
  
## S4 replacement method for signature 'XNAStringSet'  
base(x, i = 1) <- value
```

### Arguments

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
i	numeric - possibilities: 1 or 2. If 1 - 1st slots elements printed out, 2nd otherwise. In case the second element is not in the object, empty char created. This parameter is only available for XNAStringSet objects.
value	character vector applied only for setter method

### Details

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. name<- method overwrites existing name slot

### Value

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

## Examples

```
my_dic <- data.table::data.table(  
  type = c(  
    rep("base", 3),  
    rep("sugar", 2),  
    rep("backbone", 3)  
  ),  
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")  
)  
obj <- XNAString(  
  name = "b",  
  base = "GGE",  
  sugar = "FFO",  
  dictionary = my_dic  
)  
base(obj)
```

---

changeBase

*Translate base slot based on complementary bases dictionary. Base sequence in transformed using compl\_target column.*

---

## Description

Translate base slot based on complementary bases dictionary. Base sequence in transformed using compl\_target column.

## Usage

```
changeBase(compl_dict, bases)
```

## Arguments

compl_dict	complementary bases dictionary
bases	string, one or two-elements vector

## Value

string



---

complementary\_bases     *Default XNAString complementarity dictionary*

---

### Description

A dataset containing default internal XNAString dictionary with base complementary.

### Usage

```
data(complementary_bases)
```

### Format

A data.table with 6 rows and 3 variables:

**base** base symbol

**target** complementary base

**compl\_target** complementary target

### Source

RMR internal bioinformatics database (Mimir)

---

compl\_dictionary     *Compl\_dictionary setter/getter method*

---

### Description

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

### Usage

```
compl_dictionary(x, ...)
```

```
## S4 method for signature 'XNAString'  
compl_dictionary(x)
```

```
compl_dictionary(x, ...) <- value
```

```
## S4 replacement method for signature 'XNAString'  
compl_dictionary(x) <- value
```

**Arguments**

x XNAString/XNAStringSet object  
 ... optional arguments to generic function to support additional methods  
 value character vector applied only for setter method

**Details**

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. name<- method overwrites existing name slot

**Value**

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```
my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj <- XNAString(
  name = "b",
  base = "GGE",
  sugar = "FFO",
  dictionary = my_dic
)
compl_dictionary(obj)
```

---

concatDict

*Concatenate HELM-symbol custom dictionary with built-in HELM-symbol dictionary (xna\_dictionary)*


---

**Description**

Concatenate HELM-symbol custom dictionary with built-in HELM-symbol dictionary (xna\_dictionary)

**Usage**

```
concatDict(
  custom_dict,
  default_dict = xna_dictionary,
  helm_colname = "HELM",
  type_colname = "type",
  symbol_colname = "symbol"
)
```

**Arguments**

custom\_dict      custom HELM-symbol dictionary  
 default\_dict     built-in HELM-symbol dictionary (xna\_dictionary)  
 helm\_colname     helm column name in custom dictionary  
 type\_colname     type column name in custom dictionary  
 symbol\_colname   symbol column name in custom dictionary

**Value**

data.table

**Examples**

```

my_dict <- data.table::data.table(
  HELM = c("[[B]]"),
  type = c("base"),
  symbol = c("B")
)
concatDict(my_dict)

```

---

conjugate3

*Conjugate3 setter/getter method*

---

**Description**

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

**Usage**

```

conjugate3(x, ...)

## S4 method for signature 'XNAString'
conjugate3(x)

## S4 method for signature 'XNAStringSet'
conjugate3(x, i = 1)

conjugate3(x, ...) <- value

## S4 replacement method for signature 'XNAString'
conjugate3(x) <- value

## S4 replacement method for signature 'XNAStringSet'
conjugate3(x, i = 1) <- value

```

**Arguments**

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
i	numeric - possibilities: 1 or 2. If 1 - 1st slots elements printed out, 2nd otherwise. In case the second element is not in the object, empty char created. This parameter is only available for XNAStringSet objects.
value	character vector applied only for setter method

**Details**

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. `name<-` method overwrites existing name slot

**Value**

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```
my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj <- XNAString(
  name = "b",
  base = "GGE",
  sugar = "FFO",
  dictionary = my_dic
)
conjugate3(obj)
```

---

conjugate5

*Conjugate5 setter/getter method*


---

**Description**

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. `name` method extracts name slot from XNAString/XNAStringSet object.

**Usage**

```

conjugate5(x, ...)

## S4 method for signature 'XNAString'
conjugate5(x)

## S4 method for signature 'XNAStringSet'
conjugate5(x, i = 1)

conjugate5(x, ...) <- value

## S4 replacement method for signature 'XNAString'
conjugate5(x) <- value

## S4 replacement method for signature 'XNAStringSet'
conjugate5(x, i = 1) <- value

```

**Arguments**

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
i	numeric - possibilities: 1 or 2. If 1 - 1st slots elements printed out, 2nd otherwise. In case the second element is not in the object, empty char created. This parameter is only available for XNAStringSet objects.
value	character vector applied only for setter method

**Details**

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. name<- method overwrites existing name slot

**Value**

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```

my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj <- XNAString(
  name = "b",
  base = "GGE",
  sugar = "FFO",

```

```
    dictionary = my_dic
  )
  conjugate5(obj)
```

---

default_backbone	<i>Default_backbone setter/getter method</i>
------------------	--

---

## Description

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

## Usage

```
default_backbone(x, ...)
```

```
## S4 method for signature 'XNAString'
```

```
default_backbone(x)
```

```
## S4 method for signature 'XNAStringSet'
```

```
default_backbone(x)
```

```
default_backbone(x, ...) <- value
```

```
## S4 replacement method for signature 'XNAString'
```

```
default_backbone(x) <- value
```

## Arguments

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
value	character vector applied only for setter method

## Details

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. name<- method overwrites existing name slot

## Value

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```

my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj <- XNAString(
  name = "b",
  base = "GGE",
  default_sugar = 'F',
  default_backbone = 'X',
  dictionary = my_dic
)
default_backbone(obj)

```

---

default\_sugar

*Default\_sugar setter/getter method*


---

**Description**

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

**Usage**

```

default_sugar(x, ...)

## S4 method for signature 'XNAString'
default_sugar(x)

## S4 method for signature 'XNAStringSet'
default_sugar(x)

default_sugar(x, ...) <- value

## S4 replacement method for signature 'XNAString'
default_sugar(x) <- value

```

**Arguments**

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
value	character vector applied only for setter method

**Details**

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. `name<-` method overwrites existing name slot

**Value**

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```
my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj <- XNAString(
  name = "b",
  base = "GGE",
  default_sugar = 'F',
  default_backbone = 'X',
  dictionary = my_dic
)
default_sugar(obj)
```

---

dictionary

*Dictionary setter/getter method*

---

**Description**

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. `name` method extracts name slot from XNAString/XNAStringSet object.

**Usage**

```
dictionary(x, ...)
```

```
## S4 method for signature 'XNAString'
dictionary(x)
```

```
dictionary(x, ...) <- value
```

```
## S4 replacement method for signature 'XNAString'
dictionary(x) <- value
```



**Arguments**

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
value	character vector applied only for setter method

**Details**

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. `name<-` method overwrites existing name slot

**Value**

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```
my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj <- XNAString(
  name = "b",
  base = "GGE",
  sugar = "FFO",
  dictionary = my_dic
)
dictionary(obj)
```

---

`dinucleotideFrequency` *XNADinucleotideFrequencyFun* returns double letters frequency for a given object in base, sugar or backbone slot

---

**Description**

`XNADinucleotideFrequencyFun` returns double letters frequency for a given object in base, sugar or backbone slot

`XNADinucleotideFrequency` method returns dinucleotide frequency for a given object. It works for 3 slots: base, sugar and backbone. If `matrix_nbr` equals 1, dinucleotide frequency for the first elements in the slot is returned. Double letters can be given as argument, otherwise unique double letters in object's dictionary are in use.

**Usage**

```

XNADinucleotideFrequencyFun(
  obj,
  slot,
  double_letters = NA,
  matrix_nbr = 1,
  as.prob = FALSE,
  base_only = FALSE
)

XNADinucleotideFrequency(
  obj,
  slot,
  double_letters = NA,
  matrix_nbr = 1,
  as.prob = FALSE,
  base_only = FALSE,
  ...
)

## S4 method for signature 'XNAString'
XNADinucleotideFrequency(
  obj,
  slot,
  double_letters = NA,
  matrix_nbr = 1,
  as.prob = FALSE,
  base_only = FALSE
)

## S4 method for signature 'XNAStringSet'
XNADinucleotideFrequency(
  obj,
  slot,
  double_letters = NA,
  matrix_nbr = 1,
  as.prob = FALSE,
  base_only = FALSE
)

```

**Arguments**

obj	XNAString or XNAStringSet class
slot	string (slot name: base, sugar or backbone)
double_letters	string (or string vector) - double letters
matrix_nbr	numeric (1 or 2, if 1 - first slot's element is use, if 2 - 2nd element in slot)
as.prob	logical - if TRUE frequency returned as probability of occurrence

base\_only        logical - if TRUE, frequency checked for 'A', 'C', 'G', 'T', other  
 ...             optional arguments to generic function to support additional methods

### Value

matrix (frequency matrix for a given slot)

### Examples

```
my_dic <-
data.table::data.table(
  type = c(rep("base", 3), rep("sugar", 2), rep("backbone", 3)),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
xnastring_obj <- XNAString(
  name = "b",
  base = c("GGEG"),
  sugar = c("FFO"),
  dictionary = my_dic
)
XNAString::XNADinucleotideFrequency(
  obj = xnastring_obj,
  slot = "base",
  matrix_nbr = 1
)
```

---

dt2Set	<i>Function which creates XNAStringSet object from table with base, sugar and backbone columns.</i>
--------	---

---

### Description

Function which creates XNAStringSet object from table with base, sugar and backbone columns.

### Usage

```
dt2Set(
  table,
  col.base = "base",
  col.sugar = "sugar",
  col.backbone = "backbone",
  col.target = "target",
  default_sugar = NA,
  default_backbone = NA,
  compl_dict = complementary_bases
)
```

**Arguments**

table	data.table or data.frame (must include base, sugar and backbone columns)
col.base	character (name of base column)
col.sugar	character (name of sugar column)
col.backbone	character (name of backbone column)
col.target	character (name of target column)
default_sugar	character - only one letter. Will be replicated nchar(base) times
default_backbone	character - only one letter. Will be replicated nchar(base)-1 times
compl_dict	data.table with following columns: "base", "target". By default internal XNAS-tring dictionary is used

**Value**

XNAStringSet object

**Examples**

```
dt <- data.table::data.table(
  base = c("TT", "GG"),
  sugar = c("FF", "FO"),
  backbone = c("S", "S")
)
dt2Set(dt)
```

---

duplex\_structure      *Duplex\_structure setter/getter method*

---

**Description**

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

**Usage**

```
duplex_structure(x, ...)

## S4 method for signature 'XNAString'
duplex_structure(x)

## S4 method for signature 'XNAStringSet'
duplex_structure(x)

duplex_structure(x, ...) <- value

## S4 replacement method for signature 'XNAString'
duplex_structure(x) <- value
```

**Arguments**

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
value	character vector applied only for setter method

**Details**

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. name<- method overwrites existing name slot

**Value**

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```
my_dic <- data.table::data.table(  
  type = c(  
    rep("base", 3),  
    rep("sugar", 2),  
    rep("backbone", 3)  
  ),  
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")  
)  
obj <- XNAString(  
  name = "b",  
  base = "GGE",  
  sugar = "FFO",  
  dictionary = my_dic  
)  
duplex_structure(obj)
```

---

helm2String

*Translate RNA from HELM notation to multi-string notation*

---

**Description**

This function translates RNA molecules encoded in HELM notation into multi-string notation. It uses dictionary which links HELM code for base, sugar and backbone elements with symbols used in multi-string notation.

**Usage**

```
helm2String(helm, dictionary = xna_dictionary, remove_linker = TRUE)
```

**Arguments**

helm	string with HELM sequence, which contains one RNA polymer and optionally CHEM element
dictionary	data.table with following columns: "HELM", "type", "symbol". By default internal XNAString dictionary is used.
remove_linker	logical defines if linker should be clipped from RNA

**Value**

named list of strings with following elements: base, sugar, backbone, conjugate5, conjugate3

**Author(s)**

Marianna Plucinska

**Examples**

```
helm2String("RNA1{[dR](A)P.[dR](A)P.[dR](A)}$$$$V2.0")
```

---

instanceOf

*Check on an object type*

---

**Description**

Check on an object type

**Usage**

```
instanceOf(object, type)
```

**Arguments**

object	an object of any class
type	class of an object

**Value**

logical information. TRUE if object class equals type

**Examples**

```
instanceOf(1, "numeric")
```

---

listOflists2Dt	<i>Save list of lists as data.table</i>
----------------	---

---

**Description**

Save list of lists as data.table

**Usage**

```
listOflists2Dt(list_of_lists)
```

**Arguments**

list\_of\_lists list of lists that will be saved as data.table.

**Value**

data.table

**Examples**

```
nested_list <- list(  
  list(base = c("T"), sugar = c("G")),  
  list(base = c("U"), sugar = c("G"))  
)  
listOflists2Dt(nested_list)
```

---

mimir2XnaDict	<i>Reformat mimir table to XNA dictionary standards</i>
---------------	---

---

**Description**

Reformat mimir table to XNA dictionary standards

**Usage**

```
mimir2XnaDict(table, base.col, sugar.col, backbone.col)
```

**Arguments**

table	data.table or data.frame (must include "HELM", "TS_BASE_SEQ", "TS_SUGAR_SEQ" and "TS_BACKBONE_SEQ" columns)
base.col	character (base column name)
sugar.col	character (sugar column name)
backbone.col	character (backbone column name)

**Value**

data.table (written in the xna\_dictionary format)

**Examples**

```
dt <- data.table::data.table(HELM = c("[PPG]", "[fR]", "[srP]"),
  TS_BASE_SEQ = c("F", NA, NA),
  TS_SUGAR_SEQ = c(NA, NA, 'F'),
  TS_BACKBONE_SEQ = c(NA, 'S', NA))
mimir2XnaDict(dt, 'TS_BASE_SEQ', 'TS_SUGAR_SEQ', 'TS_BACKBONE_SEQ')
```

---

name	<i>Name setter/getter method</i>
------	----------------------------------

---

**Description**

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

**Usage**

```
name(x, ...)

## S4 method for signature 'XNAString'
name(x)

## S4 method for signature 'XNAStringSet'
name(x, i = 1)

name(x, ...) <- value

## S4 replacement method for signature 'XNAString'
name(x) <- value

## S4 replacement method for signature 'XNAStringSet'
name(x, i = 1) <- value
```

**Arguments**

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
i	numeric - possibilities: 1 or 2. If 1 - 1st slots elements printed out, 2nd otherwise. In case the second element is not in the object, empty char created. This parameter is only available for XNAStringSet objects.
value	character vector applied only for setter method



**Details**

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. `name<-` method overwrites existing name slot

**Value**

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```
my_dic <- data.table::data.table(  
  type = c(  
    rep("base", 3),  
    rep("sugar", 2),  
    rep("backbone", 3)  
  ),  
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")  
)  
obj <- XNAString(  
  name = "b",  
  base = "GGE",  
  sugar = "FFO",  
  dictionary = my_dic  
)  
name(obj)  
my_dic <- data.table::data.table(  
  type = c(  
    rep("base", 3),  
    rep("sugar", 2),  
    rep("backbone", 3)  
  ),  
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")  
)  
obj1 <- XNAString(  
  name = "b",  
  base = "GGE",  
  sugar = "FFO",  
  dictionary = my_dic  
)  
obj2 <- XNAString(  
  name = "b",  
  base = c("GGE", "EEE"),  
  sugar = c("FFO", "OOO"),  
  dictionary = my_dic  
)  
XNAStringSetObj <- XNAStringSet(objects = list(obj1, obj2))  
name(XNAStringSetObj)  
my_dic <- data.table::data.table(  
  type = c(  
    rep("base", 3),  
    rep("sugar", 2),  
    rep("backbone", 3)  
  )
```

```

    ),
    symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
  )
obj <- XNAString(
  name = "b",
  base = "GGE",
  sugar = "FFO",
  dictionary = my_dic
)
name(obj) <- "new_name"
my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj1 <- XNAString(
  name = "b",
  base = "GGE",
  sugar = "FFO",
  dictionary = my_dic
)
obj2 <- XNAString(
  name = "b",
  base = c("GGE", "EEE"),
  sugar = c("FFO", "OOO"),
  dictionary = my_dic
)
XNAStringSetObj <- XNAStringSet(objects = list(obj1, obj2))
name(XNAStringSetObj, 1) <- c("new1", "new2")

```

---

objects

*Objects getter method for XNAStringSet class*


---

### Description

Getter methods enable extraction of single slots from XNAStringSet objects. E.g. objects method extracts objects slot from XNAStringSet object. It is a list of XNAString objects.

### Usage

```
objects(x, ...)
```

```
## S4 method for signature 'XNAStringSet'
objects(x)
```

**Arguments**

x XNAStringSet object  
... optional arguments to generic function to support additional methods

**Value**

list of XNAString objects

**Examples**

```
my_dic <- data.table::data.table(type = c(rep('base',3),
                                         rep('sugar',2),
                                         rep('backbone',3)),
                                symbol = c('G', 'E', 'A', 'F',
                                           'O', 'S', 'B', 'X'))

obj2 <- XNAString(name = 'b',
                  base = 'GGE',
                  sugar = 'FFO',
                  dictionary = my_dic)
obj3 <- XNAString(name = 'b',
                  base = c('GGE', 'EEE'),
                  sugar = c('FFO', 'OOO'),
                  dictionary = my_dic)
XNAStringSetObj <- XNAStringSet(objects=list(obj2, obj3))
objects(XNAStringSetObj)
```

---

parseRnaHelmComponent *Parse monomers from HELM to multi-string notation*

---

**Description**

Parse monomers from HELM to multi-string notation

**Usage**

```
parseRnaHelmComponent(rna_component, dictionary = xna_dictionary)
```

**Arguments**

rna\_component list of monomers building RNA  
dictionary data.table with following columns: "HELM", "type", "symbol". By default internal XNAString dictionary is used.

**Value**

list of three strings: base, sugar, backbone

**Author(s)**

Marianna Plucinska

**Examples**

```
parseRnaHelmComponent(c("[dR](A)P", "[dR](A)P", "[dR](A)"))
```

---

predictDuplexStructure

*Compute Minimum Free Energy (MFE), and a corresponding secondary structure for two dimerized RNA sequences.*

---

**Description**

This function is a wrapper for RNAcifold from ViennaRNA package.

**Usage**

```
predictDuplexStructureFun(obj)

predictDuplexStructure(obj, ...)

## S4 method for signature 'XNAString'
predictDuplexStructure(obj)
```

**Arguments**

obj	XNAString object
...	optional arguments to generic function to support additional methods

**Value**

list (structure and mfe)

**Examples**

```
obj1 <- XNAString(
  base = "ATCG",
  sugar = "FODD",
  conjugate3 = "TAG"
)
predictDuplexStructure(obj1)
```

---

predictMfeStructure    *Prediction of MFE structure with ViennaRNA package*

---

**Description**

This function is a wrapper for RNAfold from ViennaRNA package.

**Usage**

```
predictMfeStructureFun(obj)

predictMfeStructure(obj, ...)

## S4 method for signature 'XNAString'
predictMfeStructure(obj)
```

**Arguments**

obj                    XNAString object  
...                    optional arguments to generic function to support additional methods

**Value**

character, secondary structure in dot-bracket notation

**Examples**

```
obj1 <- XNAString(
  base = "ATCG",
  sugar = "FODD",
  conjugate3 = "TAG"
)
predictMfeStructure(obj1)
```

---

reverseComplementFun    *Reverse complement sequence based on dictionary*

---

**Description**

Reverse complement sequence based on dictionary

**Usage**

```
reverseComplementFun(obj)
```

**Arguments**

obj                    XNAString object

**Value**

string with reverse complement sequence

---

secondary\_structure    *Secondary\_structure setter/getter method*

---

**Description**

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

**Usage**

```
secondary_structure(x, ...)

## S4 method for signature 'XNAString'
secondary_structure(x)

## S4 method for signature 'XNAStringSet'
secondary_structure(x)

secondary_structure(x, ...) <- value

## S4 replacement method for signature 'XNAString'
secondary_structure(x) <- value
```

**Arguments**

x                    XNAString/XNAStringSet object  
 ...                optional arguments to generic function to support additional methods  
 value              character vector applied only for setter method

**Details**

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. name<- method overwrites existing name slot

**Value**

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```
my_dic <- data.table::data.table(  
  type = c(  
    rep("base", 3),  
    rep("sugar", 2),  
    rep("backbone", 3)  
  ),  
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")  
)  
obj <- XNAString(  
  name = "b",  
  base = "GGE",  
  sugar = "FFO",  
  dictionary = my_dic  
)  
secondary_structure(obj)
```

---

seqAlphabetFrequency *Create set of functions and methods to calculate alphabet frequency in base, sugar and backbone slots*

---

**Description**

Create set of functions and methods to calculate alphabet frequency in base, sugar and backbone slots

**Usage**

```
seqAlphabetFrequency(unique_letters, seq, as.prob)
```

**Arguments**

unique\_letters string (or character) - these letters pose column names  
seq string (or character) - frequency is calculated for this string  
as.prob logical - if TRUE frequency returned as probability of occurrence

**Value**

numeric - named numeric vector

**Examples**

```
seqAlphabetFrequency(c("A", "B", "C"), c("AABA"), as.prob = FALSE)
```

---

```
seqDinucleotideFrequency
```

*Create set of functions and methods to calculate dinucleotide frequency in base, sugar and backbone slots*

---

### Description

Create set of functions and methods to calculate dinucleotide frequency in base, sugar and backbone slots

### Usage

```
seqDinucleotideFrequency(unique_sets, seq, as.prob)
```

### Arguments

unique_sets	string vector of double letters -these letters pose column names
seq	string (or character) - frequency is calculated for this string
as.prob	logical - if TRUE frequency returned as probability of occurrence

### Value

numeric - named numeric vector

### Examples

```
seqDinucleotideFrequency(c("AB", "BA", "CD"),
                          "ABABAB",
                          as.prob = FALSE)
seqDinucleotideFrequency(c("GC", "CG", "CC"),
                          "GCCG",
                          as.prob = FALSE)
```

---

```
seqVectorAlphabetFrequency
```

*seqVectorAlphabetFrequency function calculates frequency for strings vector*

---

### Description

seqVectorAlphabetFrequency function calculates frequency for strings vector

### Usage

```
seqVectorAlphabetFrequency(unique_letters, seq_vec, as.prob)
```



**Arguments**

unique\_letters string (or character) - these letters pose column names  
 seq\_vec vector of strings (or characters) - frequency will be calculated for this vector  
 as.prob logical - if TRUE frequency returned as probability of occurrence

**Value**

matrix - each row denotes frequency for a specific string of vector

**Examples**

```
seqVectorAlphabetFrequency(c("A", "B", "C"),
  c("AABA", "BBBCCC"),
  as.prob = FALSE
)
```

---

seqVectorDinucleotideFrequency

*seqVectorDinucleotideFrequency function calculates frequency for strings vector*

---

**Description**

seqVectorDinucleotideFrequency function calculates frequency for strings vector

**Usage**

```
seqVectorDinucleotideFrequency(unique_sets, seq_vec, as.prob)
```

**Arguments**

unique\_sets string vector of double letters -these letters pose column names  
 seq\_vec vector of strings (or characters) - frequency will be calculated for this vector  
 as.prob logical - if TRUE frequency returned as probability of occurrence

**Value**

matrix - each row denotes frequency for a specific string of vector

**Examples**

```
seqVectorDinucleotideFrequency(c("AB", "BA", "CD"),
  c("ABABAB", "ABABCD"),
  as.prob = FALSE)
```

---

 set2Dt

*set2Dt function - changes XNAStringSet object to data.table*


---

**Description**

set2Dt function - changes XNAStringSet object to data.table

**Usage**

```
set2Dt(obj, slots)
```

**Arguments**

obj	XNAStringSet object
slots	slots that are saved as column names (possibilities: "name", "base", "sugar", "backbone", "target", "conjugate5", "conjugate3" and "dictionary" )

**Value**

data.table

**Examples**

```
my_dic <- data.table::data.table(type = c(rep('base',3),
                                         rep('sugar',2),
                                         rep('backbone',3)),
                               symbol = c('G', 'E', 'A', 'F',
                                          'O', 'S', 'B', 'X'))

obj2 <- XNAString(name = 'b',
                 base = 'GGE',
                 sugar = 'FFO',
                 dictionary = my_dic)
obj3 <- XNAString(name = 'b',
                 base = c('GGE','EEE'),
                 sugar = c('FFO', '000'),
                 dictionary = my_dic)
XNAStringSetObj <- XNAStringSet(objects=list(obj2, obj3))
set2Dt(XNAStringSetObj, c('base', 'sugar'))

my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj2 <- XNAString(
  name = "b",
```

```

    base = "GGE",
    sugar = "FF0",
    dictionary = my_dic
  )
obj3 <- XNAString(
  name = "b",
  base = c("GGE", "EEE"),
  sugar = c("FF0", "000"),
  dictionary = my_dic
)
XNAStringSetObj <- XNAStringSet(objects = list(obj2, obj3))
set2Dt(XNAStringSetObj, c("base", "sugar"))

```

---

set2List	<i>Define method to save XNAStringSet object as a list of XNAString objects</i>
----------	---

---

## Description

Define method to save XNAStringSet object as a list of XNAString objects

## Usage

```

set2List(obj)

## S4 method for signature 'XNAStringSet'
set2List(obj)

```

## Arguments

obj                   XNAStringSet object

## Value

list of XNAString objects

## Examples

```

my_dic <- data.table::data.table(type = c(rep('base',3),
                                         rep('sugar',2),
                                         rep('backbone',3)),
                                symbol = c('G', 'E', 'A', 'F',
                                           'O', 'S', 'B', 'X'))

obj2 <- XNAString(name = 'b',
                 base = 'GGE',
                 sugar = 'FF0',
                 dictionary = my_dic)
obj3 <- XNAString(name = 'b',
                 base = c('GGE', 'EEE'),

```

```
sugar = c('FFO', '000'),
dictionary = my_dic)
XNAStringSetObj <- XNAStringSet(objects=list(obj2, obj3))
set2List(XNAStringSetObj)
```

---

siRNA_HELM	<i>siRNA_HELM function takes XNAString object and returns pairing information for base slot. Works only for double stranded molecules.</i>
------------	--

---

### Description

siRNA\_HELM function takes XNAString object and returns pairing information for base slot. Works only for double stranded molecules.

### Usage

```
siRNA_HELM(xnastring_obj)
```

### Arguments

xnastring\_obj XNAString object

### Value

string

### Examples

```
obj1 <- XNAString(
  base = c("CCCCUGCCGUGGUUCAUAA", "UUAUGAACCCACGGCAGGGGCG"),
  sugar = c("00F0F0F0F0F0F0F0F0", "FF0F0F0F0F0F0F0F0F0"),
  backbone = c("000000000000000000", "000000000000000000"),
  conjugate3 = c(""))
)

siRNA_HELM(obj1)
```

---

sugar	<i>Sugar setter/getter method</i>
-------	-----------------------------------

---

### Description

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

**Usage**

```
sugar(x, ...)
```

```
## S4 method for signature 'XNAString'
```

```
sugar(x)
```

```
## S4 method for signature 'XNAStringSet'
```

```
sugar(x, i = 1)
```

```
sugar(x, ...) <- value
```

```
## S4 replacement method for signature 'XNAString'
```

```
sugar(x) <- value
```

```
## S4 replacement method for signature 'XNAStringSet'
```

```
sugar(x, i = 1) <- value
```

**Arguments**

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
i	numeric - possibilities: 1 or 2. If 1 - 1st slots elements printed out, 2nd otherwise. In case the second element is not in the object, empty char created. This parameter is only available for XNAStringSet objects.
value	character vector applied only for setter method

**Details**

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. name<- method overwrites existing name slot

**Value**

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```
my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj <- XNAString(
  name = "b",
  base = "GGE",
  sugar = "FFO",
```

```

    dictionary = my_dic
  )
  sugar(obj)

```

---

target	<i>Target setter/getter method</i>
--------	------------------------------------

---

### Description

Getter methods enable extraction of single slots from XNAString and XNAStringSet objects. E.g. name method extracts name slot from XNAString/XNAStringSet object.

### Usage

```

target(x, ...)

## S4 method for signature 'XNAString'
target(x)

## S4 method for signature 'XNAStringSet'
target(x, i = 1)

target(x, ...) <- value

## S4 replacement method for signature 'XNAString'
target(x) <- value

## S4 replacement method for signature 'XNAStringSet'
target(x, i = 1) <- value

```

### Arguments

x	XNAString/XNAStringSet object
...	optional arguments to generic function to support additional methods
i	numeric - possibilities: 1 or 2. If 1 - 1st slots elements printed out, 2nd otherwise. In case the second element is not in the object, empty char created. This parameter is only available for XNAStringSet objects.
value	character vector applied only for setter method

### Details

Setter methods enable overwriting single slots from XNAString and XNAStringSet objects. E.g. name<- method overwrites existing name slot

### Value

vector in getter method, XNAStringSet object (with replaced name slot) in setter method

**Examples**

```
my_dic <- data.table::data.table(  
  type = c(  
    rep("base", 3),  
    rep("sugar", 2),  
    rep("backbone", 3)  
  ),  
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")  
)  
obj <- XNAString(  
  name = "b",  
  base = "GGE",  
  sugar = "FFO",  
  dictionary = my_dic  
)  
target(obj)
```

---

typedListCheck

*Check if all objects are of XNAString class and dictionaries are the same*

---

**Description**

Check if all objects are of XNAString class and dictionaries are the same

**Usage**

```
typedListCheck(object)
```

**Arguments**

object            an object of any class. An object must contain 'objects' (list type) slot

**Value**

logical information. Checks the whole list of objects, TRUE if class of all objects equals 'XNAS-tring' and their dictionaries are the same.

**Examples**

```
my_dic <- data.table::data.table(  
  type = c(  
    rep("base", 3),  
    rep("sugar", 2),  
    rep("backbone", 3)  
  ),  
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")  
)  
obj2 <- XNAString(  
  name = "b",  
  base = "GGE",  
  sugar = "FFO",  
  dictionary = my_dic  
)  
target(obj2)
```

```
name = "b",
base = "GGE",
sugar = "FFO",
dictionary = my_dic
)
obj3 <- XNAString(
  name = "b",
  base = c("GGE", "EEE"),
  sugar = c("FFO", "000"),
  dictionary = my_dic
)
XNAStringSetObj <- XNAStringSet(objects = list(obj2, obj3))
typedListCheck(XNAStringSetObj)
```

---

uniqueChars

*Utility functions useful when programming and developing XNAString class*

---

## Description

Utility functions useful when programming and developing XNAString class

## Usage

```
uniqueChars(x)
```

## Arguments

x                    A string vector

## Value

A list of vectors with unique characters found in x string

## Examples

```
uniqueChars("TRGFFTR")
uniqueChars(c("TRGFFTR", "AATGRC"))
```



---

XNAMatchPattern	<i>Finds pattern in reference sequence</i>
-----------------	--

---

### Description

This is function finding all the occurrences of a given pattern (typically short) in a (typically long) reference sequence

### Usage

```
XNAMatchPattern(  
  pattern,  
  subject,  
  target.number = 1,  
  max.mismatch = 0,  
  min.mismatch = 0,  
  with.indels = FALSE,  
  fixed = TRUE,  
  algorithm = "auto"  
)  
  
## S4 method for signature 'XNAString,character'  
XNAMatchPattern(  
  pattern,  
  subject,  
  target.number = 1,  
  max.mismatch = 0,  
  min.mismatch = 0,  
  with.indels = FALSE,  
  fixed = TRUE,  
  algorithm = "auto"  
)  
  
## S4 method for signature 'XNAString,XString'  
XNAMatchPattern(  
  pattern,  
  subject,  
  target.number = 1,  
  max.mismatch = 0,  
  min.mismatch = 0,  
  with.indels = FALSE,  
  fixed = TRUE,  
  algorithm = "auto"  
)
```

### Arguments

pattern            XNAString object with non-empty target slot

subject	string or DNASTring object
target.number	numeric - if target is a multi-element vector, then specify which element in use. 1 is the default
max.mismatch	The maximum number of mismatching letters allowed. If non-zero, an algorithm that supports inexact matching is used.
min.mismatch	The minimum number of mismatching letters allowed. If non-zero, an algorithm that supports inexact matching is used.
with.indels	If TRUE then indels are allowed. In that case, min.mismatch must be 0 and max.mismatch is interpreted as the maximum "edit distance" allowed between the pattern and a match. Note that in order to avoid pollution by redundant matches, only the "best local matches" are returned. Roughly speaking, a "best local match" is a match that is locally both the closest (to the pattern P) and the shortest.
fixed	If TRUE (the default), an IUPAC ambiguity code in the pattern can only match the same code in the subject, and vice versa. If FALSE, an IUPAC ambiguity code in the pattern can match any letter in the subject that is associated with the code, and vice versa.
algorithm	One of the following: "auto", "naive-exact", "naive-inexact", "boyer-moore", "shift-or" or "indels".

### Value

an [XStringViews](#) object for matchPattern.

### Examples

```
s1 <-
XNAString::XNAString(
  base = Biostrings::DNASTring("GCGGAGAGAGCACAGATACA"),
  sugar = "FOODDDDDDDDDDDDDDDDD",
  target = Biostrings::DNASTringSet("GCGGAGAGAGCACAGATACA")
)
XNAString::XNAMatchPattern(
  s1,
  "GCGGAGAGAGCACAGATACAGCGGAGAGAGCACAGATACA"
)
```

---

XNAMatchPDict

*Find set of patterns in reference sequence*

---

### Description

This is function finding all the occurrences of a given set of patterns (typically short) in a (typically long) reference sequence

**Usage**

```

XNAMatchPDict(
  pdict,
  subject,
  max.mismatch = 0,
  min.mismatch = 0,
  with.indels = FALSE,
  fixed = TRUE,
  algorithm = "auto",
  verbose = FALSE
)

## S4 method for signature 'XNAString,character'
XNAMatchPDict(
  pdict,
  subject,
  max.mismatch = 0,
  min.mismatch = 0,
  with.indels = FALSE,
  fixed = TRUE,
  algorithm = "auto",
  verbose = FALSE
)

## S4 method for signature 'XNAString,XString'
XNAMatchPDict(
  pdict,
  subject,
  max.mismatch = 0,
  min.mismatch = 0,
  with.indels = FALSE,
  fixed = TRUE,
  algorithm = "auto",
  verbose = FALSE
)

```

**Arguments**

<code>pdict</code>	XNAString object, target slot taken as pdict object from Biostrings
<code>subject</code>	string containing sequence
<code>max.mismatch</code>	The maximum number of mismatching letters allowed. If non-zero, an algorithm that supports inexact matching is used.
<code>min.mismatch</code>	The minimum number of mismatching letters allowed. If non-zero, an algorithm that supports inexact matching is used.
<code>with.indels</code>	If TRUE then indels are allowed. In that case, <code>min.mismatch</code> must be 0 and <code>max.mismatch</code> is interpreted as the maximum "edit distance" allowed between the pattern and a match. Note that in order to avoid pollution by redundant

	matches, only the "best local matches" are returned. Roughly speaking, a "best local match" is a match that is locally both the closest (to the pattern P) and the shortest.
fixed	If TRUE (the default), an IUPAC ambiguity code in the pattern can only match the same code in the subject, and vice versa. If FALSE, an IUPAC ambiguity code in the pattern can match any letter in the subject that is associated with the code, and vice versa.
algorithm	One of the following: "auto", "naive-exact", "naive-inexact", "boyer-moore", "shift-or" or "indels".
verbose	TRUE or FALSE.

**Value**

an [MIndex](#) object of length M, and countPDict an integer vector of length M.

**Examples**

```
s2 <-
XNAString::XNAString(
  base = "GCGGAGAGACACAGATACA",
  sugar = "FOODDDDDDDDDDDDDDDDD",
  target = Biostrings::DNAStrSet(c(
    "GCGGAGAGAGACACAGATACA", "GGCGGAGAGACACAGATACA"
  ))
)
o <- XNAString::XNAMatchPDict(
  s2,
  "GGCGGAGAGACACAGATACAGGGCGGAGAGACACAGATACCGGAGAGACACAGATACA"
)
```

---

xnaObj2Dt

*xnaObj2Dt function - changes XNAString object to data.table*


---

**Description**

xnaObj2Dt function - changes XNAString object to data.table

**Usage**

```
xnaObj2Dt(obj, slots)
```

**Arguments**

obj	XNAString object
slots	slots that are saved as column names (possibilities: "name", "base", "sugar", "backbone", "target", "conjugate5", "conjugate3" and "dictionary" )

**Value**

data.table

---

XNAPairwiseAlignment *Pairwise alignment methods for XNAString object*


---

**Description**

This function performs pairwise alignment for sequences stored in target slot of XNAString object with subject

**Usage**

```
XNAPairwiseAlignment(pattern, subject, ...)

## S4 method for signature 'XNAString,character'
XNAPairwiseAlignment(
  pattern,
  subject,
  type = "global",
  substitutionMatrix = NULL,
  fuzzyMatrix = NULL,
  gapOpening = 10,
  gapExtension = 4,
  scoreOnly = FALSE
)
```

**Arguments**

pattern	XNAString object, pattern taken from target slot.
subject	a character vector of length 1, an XString, or an XStringSet object of length 1.
...	optional arguments to generic function to support additional methods
type	type of alignment. One of "global", "local", "overlap", "global-local", and "local-global" where "global" = align whole strings with end gap penalties, "local" = align string fragments, "overlap" = align whole strings without end gap penalties, "global-local" = align whole strings in pattern with consecutive subsequence of subject, "local-global" = align consecutive subsequence of pattern with whole strings in subject.
substitutionMatrix	substitution matrix representing the fixed substitution scores for an alignment. It cannot be used in conjunction with patternQuality and subjectQuality arguments.
fuzzyMatrix	fuzzy match matrix for quality-based alignments. It takes values between 0 and 1; where 0 is an unambiguous mismatch, 1 is an unambiguous match, and values in between represent a fraction of "matchiness".

gapOpening	the cost for opening a gap in the alignment.
gapExtension	the incremental cost incurred along the length of the gap in the alignment.
scoreOnly	logical to denote whether or not to return just the scores of the optimal pairwise alignment.

**Value**

an instance of class `PairwiseAlignments`

**Examples**

```
mat <-
  pwalgn::nucleotideSubstitutionMatrix(
    match = 1,
    mismatch = -3,
    baseOnly = TRUE
  )
s1 <-
  XNAString::XNAString(
    base = "GCGGAGAGAGCACAGATACA",
    sugar = "FODDDDDDDDDDDDDDDDD",
    target = Biostrings::DNAStrSet("GCGGAGAGAGCACAGATACA")
  )

  XNAString::XNAPairwiseAlignment(s1,
                                   "ACCCACACACACACACACAC",
                                   "global",
                                   substitutionMatrix = mat
  )
```

---

XNAReverseComplement *Reverse complement sequence based on dictionary*

---

**Description**

Reverse complement sequence based on dictionary

**Usage**

```
XNAReverseComplement(obj, ...)
```

## S4 method for signature 'XNAString'

```
XNAReverseComplement(obj)
```

**Arguments**

obj XNAString object

... optional arguments to generic function to support additional methods

**Value**

string with reverse complement sequence

**Examples**

```
my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj <- XNAString(
  name = "b",
  base = "GGE",
  sugar = "FFO",
  dictionary = my_dic
)
XNAReverseComplement(obj)
```

---

XNAString-class

*Development of XNAString class aims at enabling efficient manipulation of modified oligonucleotide sequences. The class consists of the following slots: name, base, sugar, backbone, target, conjugate5, conjugate3, secondary\_structure, duplex\_structure, dictionary (HELM-string dictionary), compl\_dictionary.*

---

**Description**

The package inherits some of the functionalities from Biostrings package. In contrary to Biostrings sequences, XNAString classes allow for description of base sequence, sugar and backbone in a single object. XNAString is able to capture single stranded oligonucleotides, siRNAs, PNAs, shRNAs, gRNAs and synthetic mRNAs, and enable users to apply sequence-manipulating Bioconductor packages to their analysis. XNAString can read and write a HELM notation, compute alphabet frequency, align and match targets.

**Usage**

```
XNAString(
  name,
  base,
  sugar,
  backbone,
  target,
  conjugate5,
  conjugate3,
  secondary_structure,
```

```

    duplex_structure,
    dictionary,
    compl_dictionary,
    default_sugar,
    default_backbone
)

## S4 method for signature 'XNAString'
show(object)

## S4 method for signature 'XNAString'
initialize(
  .Object,
  name,
  base,
  sugar,
  backbone,
  target,
  conjugate5,
  conjugate3,
  secondary_structure,
  duplex_structure,
  dictionary,
  compl_dictionary,
  default_sugar,
  default_backbone
)

seqtype(x)

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

```

### Arguments

name	string (or character)
base	string (or character), RNAString, RNAStringSet, DNAString or DNAStringSet
sugar	string (or character)
backbone	string (or character)
target	DNAStringSet, DNAString or character
conjugate5	string (or character)
conjugate3	string (or character)
secondary_structure	list
duplex_structure	list



dictionary	data.table with following columns: "HELM", "type", "symbol". By default internal XNAString dictionary is used.
compl_dictionary	data.table with following columns: "base", "target". By default internal XNAString dictionary is used
default_sugar	character, a single letter which will be replicated in sugar slot as default value
default_backbone	character, a single letter which will be replicated in backbone slot as default value
object	XNAString object
.Object	XNAString object
x	A single string specifying the type of sequences

**Value**

Object which consists of name, base, sugar, backbone, target, conjugate5, conjugate3, secondary\_structure, duplex\_structure, dictionary, compl\_dictionary.

**Author(s)**

Anna Gorska

**Examples**

```
obj1 <- XNAString(
  base = "ATCG",
  sugar = "FODD",
  conjugate3 = "TAG"
)
obj2 <- XNAString(
  base = "ATCG",
  sugar = "FODD",
  backbone = "SBB"
)
str(obj2)
name(obj2) <- 'a'
base(obj2) <- 'ATTT'
sugar(obj2) <- 'LMFF'
backbone(obj2) <- 'BAB'
conjugate5(obj2) <- 'TFJSJG'
conjugate3(obj2) <- 'ARTSS'
my_dic <- data.table::data.table(type = c(rep('base',3),
                                         rep('sugar',2),
                                         rep('backbone',3)),
                                symbol = c('G', 'E', 'A', 'F',
                                           'O', 'S', 'B', 'X'))
obj1 <- XNAString(base = 'AAE',
                 sugar = 'FFO',
                 backbone='SB',
                 dictionary = my_dic)
```

```
obj2 <- XNAString(base = c('EAA', 'AAAA'),
                 sugar = c('FF0', '0000'),
                 name = c('a'),
                 conjugate5 = c('TTT'),
                 dictionary = my_dic)

my_dic <- data.table::data.table(
  type = c(
    rep("base", 3),
    rep("sugar", 2),
    rep("backbone", 3)
  ),
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")
)
obj1 <- XNAString(
  base = "AAE",
  sugar = "FF0",
  backbone = "SB",
  dictionary = my_dic
)
obj2 <- XNAString(
  base = c("EAA", "AAAA"),
  sugar = c("FF0", "0000"),
  name = c("a"),
  conjugate5 = c("TTT"),
  dictionary = my_dic
)
```

---

XNAString2XNAStringSet

*XNAString2XNAStringSet* function - changes XNAString object to XNAStringSet

---

### **Description**

XNAString2XNAStringSet function - changes XNAString object to XNAStringSet

### **Usage**

```
XNAString2XNAStringSet(XNAString_obj)
```

### **Arguments**

XNAString\_obj XNAString object

### **Value**

XNAStringSet object

---

xnastringClassUnions    *setClassUnion definitions*

---

### Description

setClassUnion definitions used in XNAString class. charOrDNAOrRNA consists of character, DNAString, RNAString, DNAStringSet, RNAStringSet. charOrDNA consists of character, DNAS-tring, DNAStringSet

---

xnastringElementsNumber

*Function which checks if XNAString object satisfies predefined slots length*

---

### Description

Function which checks if XNAString object satisfies predefined slots length

### Usage

```
xnastringElementsNumber(  
  xnastring_obj,  
  cond_name = "==1",  
  cond_base,  
  cond_sugar,  
  cond_backbone,  
  cond_target = ">0",  
  cond_conj5 = "==1",  
  cond_conj3 = "==1"  
)
```

### Arguments

xnastring_obj	XNAString object
cond_name	allowed name elements in object
cond_base	allowed base elements in object
cond_sugar	allowed sugar elements in object
cond_backbone	allowed backbone elements in object
cond_target	allowed target elements in object
cond_conj5	allowed conj5 elements in object
cond_conj3	allowed conj3 elements in object

**Value**

logical

**Examples**

```
obj <- XNAString(
  base = c("EAA", "AAA"),
  sugar = c("FF0", "000"),
  name = c("a"),
  conjugate5 = c("TTT")
)
xnastringElementsNumber(obj,
  cond_name = "=="1",
  cond_base = "%in% c(1,2)",
  cond_sugar = "%in% c(1,2)",
  cond_backbone = "%in% c(1,2)",
  cond_target = ">0",
  cond_conj5 = "=="1",
  cond_conj = "=="1"
)
```

---

XNAStringFromHelm      *Create XNAString object from HELM - user interface*

---

**Description**

Create XNAString object from HELM - user interface

**Usage**

```
XNAStringFromHelm(
  helm,
  name = NA_character_,
  dictionary = xna_dictionary,
  compl_dictionary = complementary_bases,
  remove_linker = TRUE
)
```

**Arguments**

helm	string (or strings vector) with HELM sequence, which contains one RNA polymer and optionally CHEM element
name	character (or character vector)
dictionary	data.table with following columns: "HELM", "type", "symbol". By default internal XNAString dictionary is used.
compl_dictionary	data.table with following columns: "base", "target". By default internal XNAString dictionary is used
remove_linker	logical defines if linker should be clipped from RNA

**Value**

XNAString object if single helm, XNAStringSet object otherwise

**Author(s)**

Marianna Plucinska

**Examples**

```
XNAStringFromHelm("RNA1{[dR](A)P.[dR](A)P.[dR](A)}$$$$V2.0")
XNAStringFromHelm("RNA1{[dR](A)P.[dR](A)P.[dR](A)}$$$$V2.0", 'name')
XNAStringFromHelm(c("RNA1{[dR](A)P.[dR](A)P.[dR](A)}$$$$V2.0",
                    "RNA1{[dR](T)P.[dR](T)P.[dR](A)}$$$$V2.0"),
                  c('name1', 'name2'))
```

---

XNAStringSet-class      *Create class which consists of XNAString objects given as a list*

---

**Description**

Create class which consists of XNAString objects given as a list

Create XNAStringSet object

Define show method

Method to extract a row/rows (either by row index or by 'name' slot) XNAStringSet object is returned.

Method to extract a single row (either by row index or by 'name' slot) XNAString object is returned.

**Usage**

```
XNAStringSet(
  objects = NA,
  base = NA,
  sugar = NA,
  backbone = NA,
  target = NA,
  col.base = "base",
  col.sugar = "sugar",
  col.backbone = "backbone",
  col.target = "target",
  default_sugar = NA,
  default_backbone = NA,
  compl_dict = complementary_bases
)

## S4 method for signature 'XNAStringSet'
```

```

show(object)

## S4 method for signature 'XNAStringSet,ANY,ANY,ANY'
x[i]

## S4 method for signature 'XNAStringSet,ANY,ANY'
x[[i]]

```

### Arguments

objects	list of XNAString objects
base	string (or character), RNAString, RNAStringSet, DNAString or DNAStringSet. In use only when objects argument is empty.
sugar	string (or character). In use only when objects argument is empty.
backbone	string (or character). In use only when objects argument is empty.
target	DNAStringSet, DNAString or character. In use only when objects argument is empty.
col.base	character (name of base column). In use only when objects argument is empty.
col.sugar	character (name of sugar column). In use only when objects argument is empty.
col.backbone	character (name of backbone column). In use only when objects argument is empty.
col.target	character (name of target column). In use only when objects argument is empty.
default_sugar	character - only one letter. Will be replicated nchar(base) times. In use only when objects argument is empty.
default_backbone	character - only one letter. Will be replicated nchar(base)-1 times. In use only when objects argument is empty.
compl_dict	data.table with following columns: "base", "target". By default internal XNAString dictionary is used. In use only when objects argument is empty.
object	XNAStringSet object
x	XNAStringSet object
i	numeric, integer, character, logical - filter needed for extraction method

### Value

XNAStringSet object

### Author(s)

Anna Gorska

## Examples

```
my_dic <- data.table::data.table(  
  type = c(  
    rep("base", 3),  
    rep("sugar", 2),  
    rep("backbone", 3)  
  ),  
  symbol = c("G", "E", "A", "F", "O", "S", "B", "X")  
)  
obj1 <- XNAString(  
  name = "a",  
  base = "GGE",  
  sugar = "FFO",  
  backbone = "SB",  
  dictionary = my_dic  
)  
obj2 <- XNAString(  
  name = "b",  
  base = "GGE",  
  sugar = "FFO",  
  dictionary = my_dic  
)  
obj3 <- XNAString(  
  name = "b",  
  base = c("GGE", "EEE"),  
  sugar = c("FFO", "OOO"),  
  dictionary = my_dic  
)  
XNAStringSetObj <- XNAStringSet(objects = list(obj1, obj2, obj3))
```

---

XNAStringToHelm	<i>XNAStringToHelmFun</i> function takes XNAString object and translates base, sugar and backbone to HELM notation
-----------------	--

---

## Description

XNAStringToHelmFun function takes XNAString object and translates base, sugar and backbone to HELM notation

## Usage

```
XNAStringToHelm(xnastring_obj, dictionary = xna_dictionary)
```

## Arguments

xnastring_obj	XNAString object
dictionary	HELM-symbol dictionary

**Value**

string (HELM notation)

**Examples**

```
obj <- XNAString(
  base = "AAA",
  sugar = "DDD",
  backbone = "00"
)
XNAStringToHelm(obj)
```

---

XNAVmatchPattern	<i>This is function finding all the occurrences of a given pattern (typically short) in a (typically long) set of reference sequences.</i>
------------------	--

---

**Description**

This is function finding all the occurrences of a given pattern (typically short) in a (typically long) set of reference sequences.

Implementation of this method is based on vmatchPattern method from BSgenome

**Usage**

```
XNAVmatchPattern(
  pattern,
  subject,
  target.number = 1,
  max.mismatch = 0,
  min.mismatch = 0,
  with.indels = FALSE,
  fixed = TRUE,
  algorithm = "auto",
  exclude = "",
  maskList = logical(0),
  userMask = IRanges::IRangesList(),
  invertUserMask = FALSE
)

## S4 method for signature 'XNAString,character'
XNAVmatchPattern(
  pattern,
  subject,
  target.number = 1,
  max.mismatch = 0,
  min.mismatch = 0,
  with.indels = FALSE,
```



```

    fixed = TRUE,
    algorithm = "auto"
)

## S4 method for signature 'XNAString,XStringSet'
XNAVmatchPattern(
  pattern,
  subject,
  target.number = 1,
  max.mismatch = 0,
  min.mismatch = 0,
  with.indels = FALSE,
  fixed = TRUE,
  algorithm = "auto"
)

## S4 method for signature 'XNAString,BSgenome'
XNAVmatchPattern(
  pattern,
  subject,
  target.number = 1,
  max.mismatch = 0,
  min.mismatch = 0,
  with.indels = FALSE,
  fixed = TRUE,
  algorithm = "auto",
  exclude = "",
  maskList = logical(0),
  userMask = IRanges::IRangesList(),
  invertUserMask = FALSE
)

```

### Arguments

pattern	XNAString object with non-empty target slot
subject	string, string vector or DNAString / DNAStringSet / chromosome from BSgenome object
target.number	numeric - if target is a multi-element vector, then specify which element in use. 1 is the default
max.mismatch	The maximum number of mismatching letters allowed. If non-zero, an algorithm that supports inexact matching is used.
min.mismatch	The minimum number of mismatching letters allowed. If non-zero, an algorithm that supports inexact matching is used.
with.indels	If TRUE then indels are allowed. In that case, min.mismatch must be 0 and max.mismatch is interpreted as the maximum "edit distance" allowed between the pattern and a match. Note that in order to avoid pollution by redundant matches, only the "best local matches" are returned. Roughly speaking, a "best

	local match" is a match that is locally both the closest (to the pattern P) and the shortest.
fixed	If TRUE (the default), an IUPAC ambiguity code in the pattern can only match the same code in the subject, and vice versa. If FALSE, an IUPAC ambiguity code in the pattern can match any letter in the subject that is associated with the code, and vice versa.
algorithm	One of the following: "auto", "naive-exact", "naive-inexact", "boyer-moore", "shift-or" or "indels".
exclude	A character vector with strings that will be used to filter out chromosomes whose names match these strings. Needed for BSParams object if subject is a chromosome object from BSgenome
maskList	A named logical vector of maskStates preferred when used with a BSgenome object. When using the bsapply function, the masks will be set to the states in this vector.
userMask	An IntegerRangesList, containing a mask to be applied to each chromosome.
invertUserMask	Whether the userMask should be inverted.

**Value**

An [MIndex](#) object for vmatchPattern.

**Examples**

```
s3 <-
XNAString::XNAString(
  base = "GCGGAGAGAGCACAGATACA",
  sugar = "FODDDDDDDDDDDDDDDDDD",
  target = Biostrings::DNASTringSet(
    c("AAAAGCTTTACAAAATCCAAGATC", "GCGGAGAGAGCACAGATACA")
  )
)
chrom <- BSgenome.Hsapiens.UCSC.hg38::BSgenome.Hsapiens.UCSC.hg38$chr1
result <- XNAString::XNAMatchPattern(s3, chrom)
```

---

xna\_dictionary

*Default XNAString dictionary*


---

**Description**

A dataset containing default internal XNAString dictionary with HELM to string translation.

**Usage**

```
data(xna_dictionary)
```

**Format**

A data.table with 20 rows and 3 variables:

**HELM** HELM sequence coding monomer

**type** if element is coding base, sugar, backbone

**symbol** single string translation of HELM

**Source**

RMR internal bioinformatics database (Mimir)

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