

Package ‘cleaver’

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Title Cleavage of Polypeptide Sequences

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Imports S4Vectors, IRanges

Suggests testthat (>= 0.8), knitr, BiocStyle (>= 0.0.14), rmarkdown,
BRAIN, UniProt.ws (>= 2.36.5)

Description In-silico cleavage of polypeptide sequences. The cleavage
rules are taken from:
http://web.expasy.org/peptide_cutter/peptidecutter_enzymes.html

License GPL (>= 3)

URL <https://github.com/sgibb/cleaver/>

BugReports <https://github.com/sgibb/cleaver/issues/>

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cleaver-package *Cleavage of polypeptide sequences*

Description

This package cleaves polypeptide sequences. It provides three functions: [cleave](#), [cleavageRanges](#) and [cleavageSites](#).

Details

The cleavage rules are taken from: https://web.expasy.org/peptide_cutter/peptidecutter_enzymes.html

Package: cleaver
License: GPL (>= 3)
URL: <https://github.com/sgibb/cleaver/>

Author(s)

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References

<https://github.com/sgibb/cleaver/>

Gasteiger E., Hoogland C., Gattiker A., Duvaud S., Wilkins M.R., Appel R.D., Bairoch A.; "Protein Identification and Analysis Tools on the ExPASy Server". (In) John M. Walker (ed): The Proteomics Protocols Handbook, Humana Press (2005).

https://web.expasy.org/peptide_cutter/peptidecutter_enzymes.html

See Also

[cleave](#), [cleavageRanges](#) and [cleavageSites](#).

cleave-methods *Cleavage of polypeptide sequences*

Description

This functions cleave polypeptide sequences. Use [cleavageSites](#) to find the cleavage sites, [cleavageRanges](#) to find the cleavage ranges and [cleave](#) to get the cleavage products.

Usage

```
## S4 method for signature 'character'
cleave(x, enzym = "trypsin", missedCleavages = 0,
       custom = NULL, unique = TRUE)

## S4 method for signature 'AAString'
cleave(x, enzym = "trypsin", missedCleavages = 0,
       custom = NULL, unique = TRUE)

## S4 method for signature 'AAStringSet'
cleave(x, enzym = "trypsin", missedCleavages = 0,
       custom = NULL, unique = TRUE)

## S4 method for signature 'character'
cleavageRanges(x, enzym = "trypsin", missedCleavages = 0,
              custom = NULL)

## S4 method for signature 'AAString'
cleavageRanges(x, enzym = "trypsin", missedCleavages = 0,
              custom = NULL)

## S4 method for signature 'AAStringSet'
cleavageRanges(x, enzym = "trypsin", missedCleavages = 0,
              custom = NULL)

## S4 method for signature 'character'
cleavageSites(x, enzym = "trypsin", custom = NULL)

## S4 method for signature 'AAString'
cleavageSites(x, enzym = "trypsin", custom = NULL)

## S4 method for signature 'AAStringSet'
cleavageSites(x, enzym = "trypsin", custom = NULL)
```

Arguments

| | |
|-----------------|---|
| x | polypeptide sequences. |
| enzym | character, cleavage rule. |
| missedCleavages | numeric, number of missed cleavages. |
| custom | character, of length 1 or 2. Could be used to define own cleavage rules. The first element would be the pattern and the optional second element would be an exception (non-cleavage) pattern. Perl-like regular expressions are supported, see gregexpr for details. If custom is set the enzym is ignored. |
| unique | logical, if TRUE all duplicated cleavage products per peptide are removed. |

Details

The cleavage rules are taken from: https://web.expasy.org/peptide_cutter/peptidecutter_enzymes.html

Cleavage rules (cleavage between P1 and P1'):

| Rule name | P4 | P3 | P2 | P1 | P1' |
|----------------------------|-----------------|-----------|-----------|-------------------|-----------------|
| arg-c proteinase | - | - | - | R | - |
| asp-n endopeptidase | - | - | - | - | D |
| bnps-skatole-c | - | - | - | W | - |
| caspase1 | F,W,Y,L | - | H,A,T | D | not P,E,D,Q,K,R |
| caspase2 | D | V | A | D | not P,E,D,Q,K,R |
| caspase3 | D | M | Q | D | not P,E,D,Q,K,R |
| caspase4 | L | E | V | D | not P,E,D,Q,K,R |
| caspase5 | L,W | E | H | D | - |
| caspase6 | V | E | H,I | D | not P,E,D,Q,K,R |
| caspase7 | D | E | V | D | not P,E,D,Q,K,R |
| caspase8 | I,L | E | T | D | not P,E,D,Q,K,R |
| caspase9 | L | E | H | D | - |
| caspase10 | I | E | A | D | - |
| chymotrypsin-high | - | - | - | F,Y | not P |
| | - | - | - | W | not M,P |
| chymotrypsin-low | - | - | - | F,L,Y | not P |
| | - | - | - | W | not M,P |
| | - | - | - | M | not P,Y |
| | - | - | - | H | not D,M,P,W |
| clostripain | - | - | - | R | - |
| cnbr | - | - | - | M | - |
| enterokinase | D,E | D,E | D,E | K | - |
| factor xa | A,F,G,I,L,T,V,M | D,E | G | R | - |
| formic acid | - | - | - | D | - |
| glutamyl endopeptidase | - | - | - | E | - |
| granzyme-b | I | E | P | D | - |
| hydroxylamine | - | - | - | N | G |
| iodosobenzoic acid | - | - | - | W | - |
| lysc | - | - | - | K | - |
| lysn | - | - | - | - | K |
| lysarginase | - | - | - | - | K,R |
| neutrophil elastase | - | - | - | A,V | - |
| ntcb | - | - | - | - | C |
| pepsin1.3 | - | not H,K,R | not P | not R | F,L |
| pepsin | - | not H,K,R | not P | not R | F,L,W,Y |
| | - | not H,K,R | not P | F,L,W,Y | - |
| | - | not H,K,R | not P | F,L | - |
| proline endopeptidase | - | - | not H,K,R | P | not P |
| proteinase k | - | - | - | A,E,F,I,L,T,V,W,Y | - |
| staphylococcal peptidase i | - | - | not E | E | - |
| thermolysin | - | - | - | not D,E | A,F,I,L,M,V |
| thrombin | - | - | G | R | G |

| | | | | | |
|----------------|-----------------|-----------------|---|-----|---------|
| | A,F,G,I,L,T,V,M | A,F,G,I,L,T,V,W | P | R | not D,E |
| trypsin | - | - | - | K,R | not P |
| | - | - | W | K | P |
| | - | - | M | R | P |
| trypsin-high | - | - | - | K,R | not P |
| | - | - | W | K | P |
| | - | - | M | R | P |
| trypsin-low | - | - | - | K,R | not P |
| | - | - | W | K | P |
| | - | - | M | R | P |
| trypsin-simple | - | - | - | K,R | - |

Exceptions:

| Rule name | Enzyme name | P4 | P3 | P2 | P1 | P1' | P2' |
|--------------|-------------|----|-----|----|----|-----|-----|
| trypsin | - | - | C,D | K | D | - | - |
| | | - | - | C | K | H,Y | - |
| | | - | - | C | R | K | - |
| | | - | - | R | R | H,R | - |
| trypsin-high | - | - | C,D | K | D | - | - |
| | | - | - | C | K | H,Y | - |
| | | - | - | C | R | K | - |
| | | - | - | R | R | H,R | - |

| Rule name | Enzyme name |
|---------------------|--|
| arg-c proteinase | Arg-C proteinase |
| asp-n endopeptidase | Asp-N endopeptidase |
| bnps-skatole-c | BNPS-Skatole |
| caspase1 | Caspase 1 |
| caspase2 | Caspase 2 |
| caspase3 | Caspase 3 |
| caspase4 | Caspase 4 |
| caspase5 | Caspase 5 |
| caspase6 | Caspase 6 |
| caspase7 | Caspase 7 |
| caspase8 | Caspase 8 |
| caspase9 | Caspase 9 |
| caspase10 | Caspase 10 |
| chymotrypsin-high | Chymotrypsin-high specificity (C-term to [FYW], not before P) |
| chymotrypsin-low | Chymotrypsin-low specificity (C-term to [FYWML], not before P) |
| clostripain | Clostripain (Clostridiopeptidase B) |
| cnbr | CNBr |
| enterokinase | Enterokinase |
| factor xa | Factor Xa |
| formic acid | Formic acid |

| | |
|----------------------------|--|
| glutamyl endopeptidase | Glutamyl endopeptidase |
| granzyme-b | Granzyme B |
| hydroxylamine | Hydroxylamine |
| iodosobenzoic acid | Iodosobenzoic acid |
| lysc | LysC |
| lysn | LysN |
| lysarginase | LysargiNase |
| neutrophil elastase | Neutrophil elastase |
| ntcb | NTCB (2-nitro-5-thiocyanobenzoic acid) |
| pepsin1.3 | Pepsin (pH == 1.3) |
| pepsin | Pepsin (pH > 2) |
| proline endopeptidase | Proline-endopeptidase |
| proteinase k | Proteinase K |
| staphylococcal peptidase i | Staphylococcal Peptidase I |
| thermolysin | Thermolysin |
| thrombin | Thrombin |
| trypsin | Trypsin |
| trypsin-high | Trypsin, higher specificity as defined in PeptideMass, identical to <i>trypsin</i> |
| trypsin-low | Trypsin, C-term to K/R if C-term is not P, as defined in PeptideMass |
| trypsin-simple | Trypsin, C-term to K/R, even before P, as defined in PeptideMass |

Value

cleave If *x* is a character it returns a list of the same length as *x*. Each element contains a character vector with the corresponding cleavage products of the polypeptides. If *x* is an [AAString](#) or an [AAStringSet](#) an [AAStringSet](#) or an [AAStringSetList](#) instance of the same length as *x* is returned. Each element contains an [AAString](#) or an [AAStringSet](#) instance with the corresponding cleavage products of the polypeptides.

cleavageRanges If *x* is a character it returns a list of the same length as *x*. Each element contains a two-column matrix with the start and end positions of the peptides. If *x* is an [AAString](#) or an [AAStringSet](#) instance an [IRanges](#) or an [IRangesList](#) of the same length as *x* is returned.

cleavageSites Returns a list of the same length as *x*. Each element contains an integer vector with the cleavage positions.

Overview:

| Input | cleave | cleavageRanges | cleavageSites |
|-----------------------------|---------------------------------|-----------------------------|-----------------|
| character | list of character | list of matrix | list of integer |
| AAString | AAStringSet | IRanges | list of integer |
| AAStringSet | AAStringSetList | IRangesList | list of integer |

Author(s)

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References

Gasteiger E., Hoogland C., Gattiker A., Duvaud S., Wilkins M.R., Appel R.D., Bairoch A.; "Protein Identification and Analysis Tools on the ExPASy Server". (In) John M. Walker (ed): The Proteomics Protocols Handbook, Humana Press (2005).

https://web.expasy.org/peptide_cutter/peptidecutter_enzymes.html

PeptideMass https://web.expasy.org/peptide_mass/peptide-mass-doc.html#table1

See Also

[AAString](#), [AAStringSet](#), [AAStringSetList](#), [IRanges](#), [IRangesList](#)

Examples

```
library("cleaver")

## Gastric juice peptide 1 (UniProtKB/Swiss-Prot: GAJU_HUMAN/P01358)
gaju <- "LAAGKVEDSD"

cleave(gaju, "trypsin")
# $LAAGKVEDSD
# [1] "LAAGK" "VEDSD"

cleavageRanges(gaju, "trypsin")
# $LAAGKVEDSD
#   start end
# [1,]    1  5
# [2,]    6 10

cleavageSites(gaju, "trypsin")
# $LAAGKVEDSD
# [1] 5

cleave(gaju, "trypsin", missedCleavages=1)
# $LAAGKVEDSD
# [1] "LAAGKVEDSD"

cleavageRanges(gaju, "trypsin", missedCleavages=1)
# $LAAGKVEDSD
#   start end
# [1,]    1 10

cleave(gaju, "trypsin", missedCleavages=0:1)
# $LAAGKVEDSD
# [1] "LAAGK" "VEDSD" "LAAGKVEDSD"

cleavageRanges(gaju, "trypsin", missedCleavages=0:1)
# $LAAGKVEDSD
#   start end
# [1,]    1  5
# [2,]    6 10
# [3,]    1 10
```

```

cleave(gaju, "pepsin")
# $LAAGKVEDSD
# [1] "LAAGKVEDSD"
# (no cleavage)

## use AAStrngSet
gaju <- AAStrngSet("LAAGKVEDSD")

cleave(gaju)
# AAStrngSetList of length 1
# [1] ["LAAGKVEDSD"] LAAGK VEDSD

## Beta-enolase (UniProtKB/Swiss-Prot: ENOB_THUAL/P86978)
enob <- "SITKIKAREILD"

cleave(enob, "trypsin")
# $SITKIKAREILD
# [1] "SITK" "IK" "AR" "EILD"

cleave(enob, "trypsin", missedCleavages=2)
# $SITKIKAREILD
# [1] "SITKIKAR" "IKAREILD"

cleave(enob, "trypsin", missedCleavages=0:2)
# $SITKIKAREILD
# [1] "SITK" "IK" "AR" "EILD" "SITKIK" "IKAR"
# [7] "AREILD" "SITKIKAR" "IKAREILD"

## define own cleavage rule: cleave at K
cleave(enob, custom="K")
# $SITKIKAREILD
# [1] "SITK" "IK" "AREILD"

cleavageRanges(enob, custom="K")
# $SITKIKAREILD
# start end
# [1,] 1 4
# [2,] 5 6
# [3,] 7 12

## define own cleavage rule: cleave at K but not if followed by A
cleave(enob, custom=c("K", "K(?=A)"))
# $SITKIKAREILD
# [1] "SITK" "IKAREILD"

cleavageRanges(enob, custom=c("K", "K(?=A)"))
# $SITKIKAREILD
# start end
# [1,] 1 4

```



```
# [2,]      5 12  
  
cleavageSites(enob, custom=c("K", "K(?=A)"))  
# $SITKIKAREILD  
# [1] 4
```

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