

# Package ‘cleaver’

November 20, 2024

**Version** 1.44.0

**Title** Cleavage of Polypeptide Sequences

**Maintainer** Sebastian Gibb <mail@sebastiangibb.de>

**Depends** R (>= 3.0.0), methods, Biostrings (>= 1.29.8)

**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](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/>

**LazyLoad** yes

**VignetteBuilder** knitr

**biocViews** Proteomics

**git\_url** <https://git.bioconductor.org/packages/cleaver>

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cleaver-package      *Cleavage of polypeptide sequences*

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### 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](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](https://web.expasy.org/peptide_cutter/peptidecutter_enzymes.html)

### See Also

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

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cleave-methods      *Cleavage of polypeptide sequences*

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### 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 <a href="#">gregexpr</a> 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](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
caspase2	D	V	A	D	not P,E,D,Q,K
caspase3	D	M	Q	D	not P,E,D,Q,K
caspase4	L	E	V	D	not P,E,D,Q,K
caspase5	L,W	E	H	D	-
caspase6	V	E	H,I	D	not P,E,D,Q,K
caspase7	D	E	V	D	not P,E,D,Q,K
caspase8	I,L	E	T	D	not P,E,D,Q,K
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 `AAStrng` or an `AAStrngSet` an `AAStrngSet` or an `AAStrngSetList` instance of the same length as `x` is returned. Each element contains an `AAStrng` or an `AAStrngSet` 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 `AAStrng` or an `AAStrngSet` 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	<code>cleave</code>	<code>cleavageRanges</code>	<code>cleavageSites</code>
character	list of character	list of matrix	list of integer
<code>AAStrng</code>	<code>AAStrngSet</code>	<code>IRanges</code>	list of integer
<code>AAStrngSet</code>	<code>AAStrngSetList</code>	<code>IRangesList</code>	list of integer

## Author(s)

Sebastian Gibb <mail@sebastiangibb.de>

## 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](https://web.expasy.org/peptide_cutter/peptidecutter_enzymes.html)

PeptideMass [https://web.expasy.org/peptide\\_mass/peptide-mass-doc.html#table1](https://web.expasy.org/peptide_mass/peptide-mass-doc.html#table1)

## See Also

`AAStrng`, `AAStrngSet`, `AAStrngSetList`, `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 AAStringSet
gaju <- AAStringSet("LAAGKVEDSD")

cleave(gaju)
# AAStringSetList of length 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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