

Package ‘PAAQD’

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Title PAAQD

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Depends R (>= 2.13), randomForest

Description PAAQD: Predicting immunogenicity of MHC class I binding peptides using amino acid pairwise contact potentials and quantum topological molecular similarity descriptors

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PAAQD	<i>Predicting immunogenicity of MHC class I binding peptides using amino acid pairwise contact potentials and quantum topological molecular similarity descriptors</i>
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Description

peptide immunogenicity prediction.

Usage

PAAQD (FILEPATH)

Arguments

FILEPATH The input can be vector of nonapeptide sequences or a file with ".txt" extension.
If input is a file, the content of the file must be one nonapeptide per one line

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Examples

```
PAAQD(c("AAFQSSMTK", "AAFQSSMRK", "NAFQSSMTK", "AAFQSTMTK"))
## Input is vector of nonapeptides

expath = file.path(.find.package("PAAQD"), "extdata")
## Load examples files path

PAAQD(paste(expath, "/testlist.txt", sep=''))
## Input is a ".txt" file containing one peptide per one line.
```

QuantumFea

*Encoding nonapeptide to numeric data using quantum topological
molecular similarity (QTMS) descriptors*

Description

This function is not tend to be used by user. The purpose is to encode nonapeptide sequence data to numeric data by using QTMS descriptors.

Usage

QuantumFea (TAB)

Arguments

TAB The input can be vector of nonapeptide sequences or a file with ".txt" extension.
If input is a file, the content of the file must be one nonapeptide per one line

Author(s)

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References

Hemmateenejad, B., Yousefinejad, S. and Mehdipour, A.R., 2011, Novel amino acids indices based on quantum topological molecular similarity and their application to QSAR study of peptides. Amino Acids 40, 1169-83.

Transformer*Encoding nonapeptide to numeric data*

Description

This function is not tend to be used by user. The purpose is to encode nonapeptide sequence data to numeric data by combining the information of HLA-A peptide-MHC contact site (pMHC) retrieved from the international ImMunoGeneTics information system, IMGT [Kaas and Lefranc, 2005], allele specific position scoring matrixes developed in SMMPMBEC method [Kim et al., 2009] and amino acid pairwise contact potentials from AAindex [Kawashima et al., 2008].

Usage

```
Transformer (TAB, WA9, WC, HLaseq, INSC)
```

Arguments

TAB	The nonapeptides data in tab-limited form. The first column is Peptide sequence, Class (Y= epitope, N= non epitope), Year, Aff (Affinity in logIC50), AffRaw (Affinity in the raw IC50), Unit (The using unit; nM)
WA9	Amino acid position scoring used for each allele
WC	peptide-MHC contact site (pMHC) for HLA-A
HLaseq	Amino acid sequence of specific HLA-A allele
INSC	Amino acid contact potentials used for each alleles

Author(s)

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References

Kaas Q, Lefranc MP. T cell receptor/peptide/MHC molecular characterization and standardized pMHC contact sites in IMGT/3Dstructure-DB. *In Silico Biol.* 2005;5(5-6):505-28.

Kim Y, Sidney J, Pinilla C, Sette A, Peters B. Derivation of an amino acid similarity matrix for peptide: MHC binding and its application as a Bayesian prior. *BMC Bioinformatics.* 2009;10:394.

Kawashima S, Pokarowski P, Pokarowska M, Kolinski A, Katayama T, Kanehisa M. AAindex: amino acid index database, progress report 2008. *Nucleic Acids Res.* 2008 Jan;36(Database issue):D202-5.

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