Package 'Neoantimon'

October 5, 2017

Type Package

Title Neoantimon: An R package for automatic identification of tumor-specific neoantigens from sequencing data
Version 1.1
Date 2017-06-09
Author Takanori Hasegawa
Maintainer Takanori Hasegawa <t-hasegw@ims.u-tokyo.ac.jp></t-hasegw@ims.u-tokyo.ac.jp>
Description This Package is develoed to calculate candidates neoantigens from Mutation Data (.vcf) requiring netMHCpan3.0, netMHCIIpan3.1, human refMrna, and, ref-Flat. If you do not have some of these files, see README.md.
License MIT + file LICENSE
VignetteBuilder knitr
Suggests knitr, rmarkdown
LazyData TRUE
Imports utils
RoxygenNote 6.0.1
R topics documented:
CopyNum
hla_table
hla_table2
MainINDELClass1
MainINDELClass2
MainMergeClass2
MainSNVClass1
MainSNVClass2
Neoantimon
RNAseq
sample
Index 13

2 hla_table

CopyNum

Prices of 50,000 round cut diamonds

Description

A dataset containing the prices and other attributes of almost 54,000 diamonds. The variables are as follows:

Usage

data(CopyNum)

Format

A data frame with 53940 rows and 10 variables

Details

• price. price in US dollars (\\$326-\\$18,823)

hla_table

Prices of 50,000 round cut diamonds

Description

A dataset containing the prices and other attributes of almost 54,000 diamonds. The variables are as follows:

Usage

```
data(hla_table)
```

Format

A data frame with 53940 rows and 10 variables

Details

• price. price in US dollars (\\$326-\\$18,823)

hla_table2

hla_table2

Prices of 50,000 round cut diamonds

Description

A dataset containing the prices and other attributes of almost 54,000 diamonds. The variables are as follows:

Usage

```
data(hla_table2)
```

Format

A data frame with 53940 rows and 10 variables

Details

• price. price in US dollars (\\$326-\\$18,823)

MainINDELClass1

Calculate Neoantigen Candidates on Indels for MHC Class1

Description

Calculate Neoantigen Candidates on Indels for MHC Class1

hla_table;

Usage

```
MainINDELClass1(input_file, HLA_file, file_name_in_HLA_table = input_file,
  hmdir = getwd(), job_ID = "NO_JOB_ID", RNAseq_file = NA, RNA_bam = NA,
  CNV = NA, ccfp_dir = "lib/ccfp.jar", Purity = NA,
  netMHCpan_dir = "lib/netMHCpan-3.0/netMHCpan", refDNA = "lib/GRCh37.fa",
  refFlat_file = paste(hmdir, "/data/refFlat.txt", sep = ""),
  refMrna_1 = paste(hmdir, "/data/refMrna.cut1.fa", sep = ""),
  refMrna_3 = paste(hmdir, "/data/refMrna.cut3.fa", sep = ""),
  Chr_Column = 1, Mutation_Start_Column = 2, Mutation_End_Column = 3,
  Mutation_Ref_Column = 4, Mutation_Alt_Column = 5, NM_ID_Column = 10,
  Depth_Normal_Column = NA, Depth_Tumor_Column = NA,
  ambiguous_between_exon = 0, ambiguous_codon = 0, peptide_length = c(8,
  9, 10, 11, 12, 13))
```

Arguments

input_file An input file annotated by ANNOVAR (http://annovar.openbioinformatics.org/en/latest/) or other softwares to be analyzed (Required). See by data(sample_annovar.txt); sample_annovar; data(sample_genomon); sample_genomon;

HLA_file A tab separated file indicating HLA types (Required). The 1st column is input_file name, and the following columns indicate HLA types. See by data(hla_table);

4 MainINDELClass1

file_name_in_HLA_table

If the name (1st column) in HLA table is not input file, indicate the correspond-

ing name (Default=input file).

hmdir Home directory for the analysis (Default=getwd()).

job_ID Job-Id to be attached in output files (Default="NO_JOB_ID").

(Default=NA) A file including RNA expressions. The 1st, 2nd and 3rd columns RNAseq_file

> are "GeneSymbol Chr:ExonStart-ExonEnd(locus) Expression Amount", respectively. The 1st row should be any header. See by data(RNAseq.txt); RNAseq;

RNA_bam RNA bam file to calculate variant allele frequency of RNA at each mutation

(Default=NA).

CNV A file including copy number variation to calculate cancer cell fraction probabil-

ity (CCFP) (Default=NA). The format is according to ASCAT (https://www.crick.ac.uk/peter-

refMrna file to be used in constructing peptide (Default=paste(hmdir,"ib/refMrna.merge.cut3.fa",sep=

van-loo/software/ASCAT) output files. The columns are "Chromosome Position Log R segmented LogR BAF segmented BAF Copy number Minor allele Raw copy number" The 1st row should be the above header. See data(CopyNum);

head(CopyNum);

The file directory to CCFP.pl (Default="lib/ccfp.jar"). ccfp_dir

Tumor purity or tumor contents ratio required to calculate CCFP (Default=NA). Purity netMHCpan_dir The file directory to netMHCpan (Default="ib/netMHCpan-3.0/netMHCpan"). refDNA refDNA information to be used to calculate RNA VAF (Default="ib/GRCh37.fa").

refFlat_file refFlat file to be used in constructing peptide. (Default=paste(hmdir,"ib/refFlat.txt",sep="")

This file is automaticalluy generated by Main_Preparation.sh

refMrna file to be used in constructing peptide (Default=paste(hmdir,"ib/refMrna.merge.cut1.fa",sep= refMrna 1

This file is automaticalluy generated by Main_Preparation.sh

This file is automaticalluy generated by Main_Preparation.sh

Chr Column The column number describing Chromosome number in input file (Default=1).

Mutation_Start_Column

The column number describing Mutation Start Position in input_file (Default=2)

Mutation_End_Column

refMrna_3

The column number describing Mutation End Position in input_file (Default=3).

Mutation_Ref_Column

The column number describing Mutation Ref in input file (Default=4).

Mutation_Alt_Column

The column number describing Mutation Alt in input_file (Default=5).

The column number describing NM IDs in input_file (Default=10). NM_ID_Column

Depth_Normal_Column

The column number describing the read count from normal cells (Default = NA)

Depth_Tumor_Column

The column number describing the read count from tumor cells (Default = NA)

ambiguous_between_exon

The maximum number to permit the differences between Exon-Lengths from refFlat and refMrna (Default=0).

ambiguous_codon

The maximum number to permit the differences between inputfile- and refMrnaoriented translation START/END position (Default=0).

peptide_length Peptide Length to be generated (Default=8,9,10,11,12,13).

MainINDELClass2 5

Value

void (Calculated Neoantigen Files will be generated as .tsv files.)

MainINDELClass2

Calculate Neoantigen Candidates on Indels for MHC Class2

Description

Calculate Neoantigen Candidates on Indels for MHC Class2

Usage

```
MainINDELClass2(input_file, HLA_file, file_name_in_HLA_table = input_file,
  hmdir = getwd(), job_ID = "NO_JOB_ID", RNAseq_file = NA, RNA_bam = NA,
  CNV = NA, ccfp_dir = "lib/ccfp.jar", Purity = NA,
  netMHCpan_dir = "lib/netMHCIIpan-3.1/netMHCIIpan",
  refDNA = "lib/GRCh37.fa", refFlat_file = paste(hmdir, "/data/refFlat.txt",
  sep = ""), refMrna_1 = paste(hmdir, "/data/refMrna.cut1.fa", sep = ""),
  refMrna_3 = paste(hmdir, "/data/refMrna.cut3.fa", sep = ""),
  Chr_Column = 1, Mutation_Start_Column = 2, Mutation_End_Column = 3,
  Mutation_Ref_Column = 4, Mutation_Alt_Column = 5, NM_ID_Column = 10,
  Depth_Normal_Column = NA, Depth_Tumor_Column = NA,
  ambiguous_between_exon = 0, ambiguous_codon = 0, peptide_length = c(15))
```

Arguments

input_file An input file annotated by ANNOVAR (http://annovar.openbioinformatics.org/en/latest/)

or other softwares to be analyzed (Required). See by data(sample_annovar.txt);

sample_annovar; data(sample_genomon); sample_genomon;

HLA_file A tab separated file indicating HLA types (Required). The 1st column is in-

put file name, and the following columns indicate HLA types. See by data(hla table2);

hla table2;

file_name_in_HLA_table

If the name (1st column) in HLA table is not input_file, indicate the correspond-

ing name (Default=input_file).

hmdir Home directory for the analysis (Default=getwd()).

job_ID Job-Id to be attached in output files (Default="NO_JOB_ID").

RNAseq_file (Default=NA) A file including RNA expressions. The 1st, 2nd and 3rd columns

are "GeneSymbol Chr:ExonStart-ExonEnd(locus) Expression Amount", respectively. The 1st row should be any header. See by data(RNAseq.txt); RNAseq;

RNA_bam RNA bam file to calculate variant allele frequency of RNA at each mutation

(Default=NA).

CNV A file including copy number variation to calculate cancer cell fraction probabil-

ity (CCFP) (Default=NA). The format is according to ASCAT (https://www.crick.ac.uk/peter-

van-loo/software/ASCAT) output files. The columns are "Chromosome Position Log R segmented LogR BAF segmented BAF Copy number Minor allele Raw copy number" The 1st row should be the above header. See data(CopyNum);

head(CopyNum);

6 MainMergeClass1

ccfp_dir The file directory to CCFP.pl (Default="lib/ccfp.jar").

Tumor purity or tumor contents ratio required to calculate CCFP (Default=NA). Purity The file directory to netMHCpan (Default="lib/netMHCpan-3.0/netMHCpan"). netMHCpan_dir refDNA information to be used to calculate RNA VAF (Default="lib/GRCh37.fa"). refDNA

refFlat_file refFlat file to be used in constructing peptide. (Default=paste(hmdir,"lib/refFlat.txt",sep="")

This file is automaticalluy generated by Main_Preparation.sh

refMrna file to be used in constructing peptide (Default=paste(hmdir,"lib/refMrna.merge.cut1.fa",seprefMrna_1

This file is automaticalluy generated by Main_Preparation.sh

refMrna file to be used in constructing peptide (Default=paste(hmdir,"lib/refMrna.merge.cut3.fa",seprefMrna_3

This file is automaticalluy generated by Main_Preparation.sh

Chr_Column The column number describing Chromosome number in input file (Default=1).

Mutation_Start_Column

The column number describing Mutation Start Position in input_file (Default=2)

Mutation_End_Column

The column number describing Mutation End Position in input_file (Default=3).

Mutation_Ref_Column

The column number describing Mutation Ref in input_file (Default=4).

Mutation_Alt_Column

The column number describing Mutation Alt in input_file (Default=5).

The column number describing NM IDs in input file (Default=10). NM ID Column

Depth_Normal_Column

The column number describing the read count from normal cells (Default = NA)

Depth_Tumor_Column

The column number describing the read count from tumor cells (Default = NA)

ambiguous_between_exon

The maximum number to permit the differences between Exon-Lengths from refFlat and refMrna (Default=0).

ambiguous_codon

The maximum number to permit the differences between inputfile- and refMrnaoriented translation START/END position (Default=0).

peptide_length Peptide Length to be generated (Default=15 in HLA Class2).

Value

void (Calculated Neoantigen Files will be generated as .tsv files.)

MainMergeClass1

Merge Results from MainSnvClass1.R

Description

Merge Results from MainSnvClass1.R

Usage

```
MainMergeClass1(hmdir = getwd(), input_dir, input_file_prefix,
  Tumor_RNA_BASED_ON_DNA = TRUE, INDEL = FALSE)
```

MainMergeClass2 7

Arguments

hmdir Home directory for the analysis (Default=getwd()).

input_dir Directory storing netMHCpan Results (Required).

input_file_prefix

File prefix of netMHCpan Results (Required). If you have "sample_annovar.txt.NO_JOB_ID.HLACL please set "sample_annovar", "sample_annovar.txt" or "sample_annovar.txt.NO_JOB_ID".

Tumor_RNA_BASED_ON_DNA

In calculating tumor specific RNA expression, TRUE uses variant allele fre-

quency on DNA. Otherwise, use VAF on RNA (Default=TRUE).

INDEL If the targeting results are generated from Indels, Please check TRUE.

Value

void (Calculated Neoantigen Files will be generated as .tsv files.)

MainMergeClass2

Merge Results from MainSnvClass2.R

Description

Merge Results from MainSnvClass2.R

Usage

```
MainMergeClass2(hmdir = getwd(), input_dir, input_file_prefix,
  Tumor_RNA_BASED_ON_DNA = TRUE, INDEL = FALSE)
```

Arguments

hmdir Home directory for the analysis (Default=getwd()).

input_dir Directory storing netMHCpan Results (Required).

input_file_prefix

File prefix of netMHCpan Results (Required). If you have "sample_annovar.txt.NO_JOB_ID.HLACL please set "sample_annovar", "sample_annovar.txt" or "sample_annovar.txt.NO_JOB_ID".

Tumor_RNA_BASED_ON_DNA

In calculating tumor specific RNA expression, TRUE uses variant allele fre-

quency on DNA. Otherwise, use VAF on RNA (Default=TRUE).

INDEL If the targeting results are generated from Indels, Please check TRUE.

Value

void (Calculated Neoantigen Files will be generated as .tsv files.)

8 MainSNVClass1

MainSNVClass1 Calculate Neoantigen Candidates on SNVs for MHC Class1

Description

Calculate Neoantigen Candidates on SNVs for MHC Class1

Usage

```
MainSNVClass1(input_file, HLA_file, file_name_in_HLA_table = input_file,
  hmdir = getwd(), job_ID = "NO_JOB_ID", RNAseq_file = NA, RNA_bam = NA,
  CNV = NA, ccfp_dir = "lib/ccfp.jar", Purity = NA,
  netMHCpan_dir = "lib/netMHCpan-3.0/netMHCpan", refDNA = "lib/GRCh37.fa",
  refFlat_file = paste(hmdir, "/data/refFlat.txt", sep = ""),
  refMrna_1 = paste(hmdir, "/data/refMrna.cut1.fa", sep = ""),
  refMrna_3 = paste(hmdir, "/data/refMrna.cut3.fa", sep = ""),
  Chr_Column = 1, Mutation_Start_Column = 2, Mutation_End_Column = 3,
  Mutation_Ref_Column = 4, Mutation_Alt_Column = 5, NM_ID_Column = 10,
  Depth_Normal_Column = NA, Depth_Tumor_Column = NA,
  ambiguous_between_exon = 0, ambiguous_codon = 0, peptide_length = c(8,
  9, 10, 11, 12, 13))
```

Arguments

input_file An input file annotated by ANNOVAR (http://annovar.openbioinformatics.org/en/latest/) or other softwares to be analyzed (Required). See by data(sample_annovar.txt);

sample_annovar; data(sample_genomon); sample_genomon;

HLA_file A tab separated file indicating HLA types (Required). The 1st column is in-

 $put_file\ name,\ and\ the\ following\ columns\ indicate\ HLA\ types.\ See\ by\ data(hla_table);$

hla_table;

file_name_in_HLA_table

If the name (1st column) in HLA table is not input_file, indicate the correspond-

ing name (Default=input_file).

hmdir Home directory for the analysis (Default=getwd()).

job_ID Job-Id to be attached in output files (Default="NO JOB ID").

RNAseq_file (Default=NA) A file including RNA expressions. The 1st, 2nd and 3rd columns

are "GeneSymbol Chr:ExonStart-ExonEnd(locus) Expression Amount", respectively. The 1st row should be any header. See by data(RNAseq.txt); RNAseq;

RNA_bam RNA bam file to calculate variant allele frequency of RNA at each mutation

(Default=NA).

CNV A file including copy number variation to calculate cancer cell fraction probabil-

ity (CCFP) (Default=NA). The format is according to ASCAT (https://www.crick.ac.uk/peter-

van-loo/software/ASCAT) output files. The columns are "Chromosome Position Log R segmented LogR BAF segmented BAF Copy number Minor allele Raw copy number" The 1st row should be the above header. See data(CopyNum);

head(CopyNum);

ccfp_dir The file directory to CCFP.pl (Default="lib/ccfp.jar").

Purity Tumor purity or tumor contents ratio required to calculate CCFP (Default=NA).

MainSNVClass2 9

netMHCpan_dir The file directory to netMHCpan (Default="lib/netMHCpan-3.0/netMHCpan"). refDNA refDNA information to be used to calculate RNA VAF (Default="lib/GRCh37.fa"). refFlat_file refFlat file to be used in constructing peptide. (Default=paste(hmdir, "lib/refFlat.txt", sep="") This file is automaticalluy generated by Main_Preparation.sh refMrna file to be used in constructing peptide (Default=paste(hmdir,"lib/refMrna.merge.cut1.fa",sep refMrna_1 This file is automatically generated by Main_Preparation.sh refMrna file to be used in constructing peptide (Default=paste(hmdir,"lib/refMrna.merge.cut3.fa",seprefMrna_3 This file is automaticalluy generated by Main_Preparation.sh Chr_Column The column number describing Chromosome number in input_file (Default=1). Mutation_Start_Column The column number describing Mutation Start Position in input_file (Default=2) Mutation_End_Column The column number describing Mutation End Position in input_file (Default=3). Mutation_Ref_Column The column number describing Mutation Ref in input_file (Default=4). Mutation_Alt_Column The column number describing Mutation Alt in input_file (Default=5). The column number describing NM IDs in input_file (Default=10). NM_ID_Column Depth_Normal_Column The column number describing the read count from normal cells (Default = NA) Depth_Tumor_Column The column number describing the read count from tumor cells (Default = NA) ambiguous_between_exon The maximum number to permit the differences between Exon-Lengths from refFlat and refMrna (Default=0).

ambiguous_codon

The maximum number to permit the differences between inputfile- and refMrnaoriented translation START/END position (Default=0).

 $peptide_length \ \ Peptide\ Length\ to\ be\ generated\ (Default=8,9,10,11,12,13).$

Value

void (Calculated Neoantigen Files will be generated as .tsv files.)

MainSNVClass2 Calculate Neoantigen Candidates on SNVs for MHC Class2

Description

Calculate Neoantigen Candidates on SNVs for MHC Class2

10 MainSNVClass2

Usage

```
MainSNVClass2(input_file, HLA_file, file_name_in_HLA_table = input_file,
  hmdir = getwd(), job_ID = "NO_JOB_ID", RNAseq_file = NA, RNA_bam = NA,
  CNV = NA, ccfp_dir = "lib/ccfp.jar", Purity = NA,
  netMHCpan_dir = "lib/netMHCIIpan-3.1/netMHCIIpan",
  refDNA = "lib/GRCh37.fa", refFlat_file = paste(hmdir, "/data/refFlat.txt",
  sep = ""), refMrna_1 = paste(hmdir, "/data/refMrna.cut1.fa", sep = ""),
  refMrna_3 = paste(hmdir, "/data/refMrna.cut3.fa", sep = ""),
  Chr_Column = 1, Mutation_Start_Column = 2, Mutation_End_Column = 3,
 Mutation_Ref_Column = 4, Mutation_Alt_Column = 5, NM_ID_Column = 10,
  Depth_Normal_Column = NA, Depth_Tumor_Column = NA,
  ambiguous_between_exon = 0, ambiguous_codon = 0, peptide_length = c(15))
```

Arguments

 $input_file$ An input file annotated by ANNOVAR (http://annovar.openbioinformatics.org/en/latest/)

or other softwares to be analyzed (Required). See by data(sample_annovar.txt);

sample_annovar; data(sample_genomon); sample_genomon;

HLA_file A tab separated file indicating HLA types (Required). The 1st column is in-

put_file name, and the following columns indicate HLA types. See by data(hla_table2);

hla table2;

file_name_in_HLA_table

refMrna_1

If the name (1st column) in HLA table is not input_file, indicate the correspond-

ing name (Default=input_file).

hmdir Home directory for the analysis (Default=getwd()).

Job-Id to be attached in output files (Default="NO_JOB_ID"). job_ID

RNAseq_file (Default=NA) A file including RNA expressions. The 1st, 2nd and 3rd columns

> are "GeneSymbol Chr:ExonStart-ExonEnd(locus) Expression Amount", respectively. The 1st row should be any header. See by data(RNAseq.txt); RNAseq;

RNA_bam RNA bam file to calculate variant allele frequency of RNA at each mutation

(Default=NA).

CNV A file including copy number variation to calculate cancer cell fraction probabil-

ity (CCFP) (Default=NA). The format is according to ASCAT (https://www.crick.ac.uk/peter-

refMrna file to be used in constructing peptide (Default=paste(hmdir,"lib/refMrna.merge.cut1.fa",sep-

van-loo/software/ASCAT) output files. The columns are "Chromosome Position Log R segmented LogR BAF segmented BAF Copy number Minor allele Raw copy number" The 1st row should be the above header. See data(CopyNum);

head(CopyNum);

ccfp_dir The file directory to CCFP.pl (Default="lib/ccfp.jar").

Tumor purity or tumor contents ratio required to calculate CCFP (Default=NA). Purity The file directory to netMHCpan (Default="lib/netMHCpan-3.0/netMHCpan"). netMHCpan_dir

refDNA refDNA information to be used to calculate RNA VAF (Default="lib/GRCh37.fa").

refFlat file refFlat file to be used in constructing peptide. (Default=paste(hmdir,"lib/refFlat.txt",sep="")

This file is automaticalluy generated by Main_Preparation.sh

This file is automaticalluy generated by Main_Preparation.sh

refMrna file to be used in constructing peptide (Default=paste(hmdir,"lib/refMrna.merge.cut3.fa",seprefMrna_3

This file is automatically generated by Main_Preparation.sh

The column number describing Chromosome number in input_file (Default=1). Chr_Column

Neoantimon 11

Mutation_Start_Column

The column number describing Mutation Start Position in input_file (Default=2)

Mutation_End_Column

The column number describing Mutation End Position in input_file (Default=3).

Mutation_Ref_Column

The column number describing Mutation Ref in input_file (Default=4).

Mutation_Alt_Column

The column number describing Mutation Alt in input_file (Default=5).

 $\label{eq:nm_ID_Column} \mbox{ MM_ID_Column number describing NM IDs in input_file (Default=10).}$

Depth_Normal_Column

 $\label{eq:column} The \ column \ number \ describing \ the \ read \ count \ from \ normal \ cells \ (Default=NA)$ $\ Depth_Tumor_Column$

 $\label{eq:count_state} The \ column \ number \ describing \ the \ read \ count \ from \ tumor \ cells \ (Default = NA) \\ ambiguous_between_exon$

The maximum number to permit the differences between Exon-Lengths from refFlat and refMrna (Default=0).

ambiguous_codon

The maximum number to permit the differences between inputfile- and refMrnaoriented translation START/END position (Default=0).

peptide_length Peptide Length to be generated (Default=15 in HLA Class2).

Value

void (Calculated Neoantigen Files will be generated as .tsv files.)

Neoantimon Neoantimon

Description

Calculate Lists of Candidate Neoantingens on SNVs and Indels to MHC Class1 and Class2

RNAseq

Prices of 50,000 round cut diamonds

Description

A dataset containing the prices and other attributes of almost 54,000 diamonds. The variables are as follows:

Usage

data(RNAseq)

Format

A data frame with 53940 rows and 10 variables

Details

• price. price in US dollars (\\$326-\\$18,823)

12 sample

sample

Prices of 50,000 round cut diamonds

Description

A dataset containing the prices and other attributes of almost 54,000 diamonds. The variables are as follows:

Usage

data(sample)

Format

A data frame with 53940 rows and 10 variables

Details

• price. price in US dollars (\\$326-\\$18,823)

Index

```
*Topic datasets
     CopyNum, \frac{2}{}
     hla_table, 2
     hla_table2, 3
     RNAseq, 11
     {\tt sample},\, \textcolor{red}{12}
{\sf CopyNum,\, \textcolor{red}{2}}
hla_table, 2
hla_table2, 3
MainINDELClass1, 3
MainINDELClass2, 5
MainMergeClass1, 6
MainMergeClass2, 7
MainSNVClass1, 8
MainSNVClass2, 9
Neoantimon, 11
Neoantimon-package (Neoantimon), 11
RNAseq, 11
sample, 12
```