## Package 'HMP16SData'

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Type Package Title 16S rRNA Sequencing Data from the Human Microbiome Project Author Lucas Schiffer < schiffer.lucas@gmail.com>, Rimsha Azhar <rimsha\_azhar@hotmail.com>, Marcel Ramos <marcel.ramos@roswellpark.org>, Ludwig Geistlinger < ludwig.geistlinger@sph.cuny.edu>, Levi Waldron < lwaldron.research@gmail.com> Maintainer Lucas Schiffer < schiffer.lucas@gmail.com> **Description** HMP16SData is a Bioconductor ExperimentData package of the Human Microbiome Project (HMP) 16S rRNA sequencing data for variable regions 1-3 and 3-5. Raw data files are provided in the package as downloaded from the HMP Data Analysis and Coordination Center. Processed data is provided as SummarizedExperiment class objects via ExperimentHub. License Artistic-2.0 **Encoding UTF-8** LazyData true **Depends** R (>= 3.6.0), SummarizedExperiment Imports AnnotationHub, assertthat, dplyr, ExperimentHub, kableExtra, knitr, magrittr, methods, readr, S4Vectors, stringr, tibble, Suggests Biobase, BiocCheck, BiocManager, BiocStyle, circlize, covr, cowplot, curatedMetagenomicData, dendextend, devtools, ggplot2, gridExtra, haven, phyloseq, rmarkdown, roxygen2, stats, biocViews ExperimentData, ExperimentHub, Homo\_sapiens\_Data, MicrobiomeData, ReproducibleResearch, SequencingData VignetteBuilder knitr URL https://github.com/waldronlab/HMP16SData BugReports https://github.com/waldronlab/HMP16SData/issues RoxygenNote 7.1.1 git\_url https://git.bioconductor.org/packages/HMP16SData git\_branch RELEASE\_3\_11

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as\_phyloseq

Coerce a SummarizedExperiment object to a phyloseq object

## Description

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The phyloseq-package provides a suite of methods for working with 16S rRNA sequencing and other microbiome data that may be of use to the users of HMP16SData. The as\_phyloseq method provides a means to easily coerce a SummarizedExperiment-class object to a phyloseq-class object.

## Usage

```
as_phyloseq(x)
```

#### **Arguments**

Х

 $A \ {\tt SummarizedExperiment-class} \ object \ from \ the \ {\tt HMP16SData} \ package$ 

#### Value

A phyloseq-class object

## **Examples**

```
V13() %>%
as_phyloseq()
```

attach\_dbGaP 3

attach\_dbGaP

Attach dbGaP metadata to a SummarizedExperiment object

#### **Description**

The National Center for Biotechnology Information (NCBI) database of Genotypes and Phenotypes (dbGaP) has extensive metadata pretaining to the HMP study. Access to this metadata is controlled and its use requires authorization by the appropriate Data Access Committee – further information is available here. Those with authorization will be able to download a dbGaP repository key and can use it to attach the controlled-access metadata to a SummarizedExperiment-class object with a single command, provided the NCBI SRA Toolkit is installed and on the user's PATH. See note below for further information.

#### Usage

```
attach_dbGaP(x, dbGaP_repository_key = "")
```

#### **Arguments**

```
x A SummarizedExperiment-class object from the HMP16SData package dbGaP_repository_key
```

A repository key downloaded from dbGaP; only required for the initial download and not needed thereafter

#### Value

A SummarizedExperiment-class object with protected metadata from dbGaP attached

#### Note

The NCBI SRA Toolkit is called internally and must be on the user's PATH or an error message will be displayed. The NCBI SRA Toolkit can readily be installed on multiple platforms following these instructions.

## See Also

```
dictionary
```

## **Examples**

```
## Not run:
V13() %>%
    attach_dbGaP(dbGaP_repository_key = "~/prj_12146.ngc")
## End(Not run)
```

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dictionary

A data dictionary describing dbGaP metadata variables

#### **Description**

A data dictionary containing descriptions of the metadata variables attached using the attach\_dbGaP method, as translated from dbGaP XLM data dictionary files.

#### Usage

dictionary

#### **Format**

A data. frame with 789 rows and 8 variables:

VARIABLE The name of the variable as it appears in SummarizedExperiment colData

**DESCRIPTION** A description of the variable

TYPE The type of variable, as specified by dbGaP

**UNITS** The units of the variable (e.g. days)

MINIMUM The smallest possible value of the variable

MAXIMUM The largest possible value of the variable

**CODED\_VALUES** The encoding of coded categorical variables, if needed

**COMMENT** Any comments from dbGaP, most pertain to gated fields

#### Source

The following dbGaP XLM data dictionary files were used to construct the data dictionary.

Data dictionary for data table pht001185.v4.p1: https://tinyurl.com/y7rgelao. No description provided by dbGaP.

Data dictionary for data table pht001193.v3.p1: https://tinyurl.com/y7at85tv. The data table contains subject data with sample information for the Global Trace Screen (GTV). Variables include the specimen type (based on 18 specimens from 6 body sites), nucleic extraction method, and sample administrative information. The Global Trace dataset will be updated when additional visits or subjects have been added.

Data dictionary for data table pht002157.v1.p1: https://tinyurl.com/y7af3arf. The Targeted Physical Forms (DTP), Medical History Screening Forms (DHX), and the Visit Documentation Forms (DVD) have been combined into a single data table. The DTP variables include measurements collected for blood pressure, pulse, body weight, height, and BMI. Variables also include physical assessment of areas/systems and the specific details of the abnormalities. Areas/Systems consist of general appearance, HEENT, cardiovascular, pulmonary, abdomen, neurological, musculoskeletal, and extremities. The DHX variables include data that indicate whether the subject noted medical problems in various areas/systems and the indications and specifications of medical problems. Areas/Systems consist of HEENT, cardiovascular, pulmonary, GI, hepatobiliary, renal, neurologic, blood lymphatic, endocrine/metabolic, musculoskeletal, genital/reproductive, dermatologic, allergies, cancer, immunodeficiency, drug or alcohol dependence, and autoimmune disease. Data were also collected for relevant medical or surgical history, medical abnormality with ongoing treatment and presence of acute disease. The DVD variables include education level, insurance status, occupation status, tobacco usage, and visit-specific information. This visit-specific information

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pertains to subject's oral temperature, pregnancy test results, education level, insurance status, occupation, and if blood and GI specimens were collected. DTP, DHX and DVD data will be collected at each visit though not every variable was collected.

Data dictionary for data table pht001187.v3.p1: https://tinyurl.com/ych4wywl. The data table contains data that were collected from the Concomitant Medications Form (DCM). Variables include medication number and code, indication, if the medication is ongoing, and the duration of the medication.

Data dictionary for data table pht001184.v3.p1: https://tinyurl.com/y9hwfn9e. The data table contains the subject and consent group information.

Data dictionary for data table pht002158.v1.p1: https://tinyurl.com/y7jtghxv. The Demographics Form (DEM) and the Eligibility Checklist (ENR) have been combined into a single data table. The DEM variables include sociodemographic measurements such as gender, ethnicity, race, and place of birth, while the ENR variables include the enrollment/first sampling time of subjects (n=1 variable) and administrative variables (n=4 variables). Both the Medical History and Targeted Physical exams must be completed prior to the completion of the Exclusion Criteria found in the ENR form. Data derived from the Medical History (DHX) and Targeted Physical (DTP) exams can be found in EMMES\_HMP\_DTP\_DHX\_DVD dataset.

Data dictionary for data table pht002156.v1.p1: https://tinyurl.com/y7znjmak. The data table contains data that were collected from the Suppplemental Questions Form (DSU) upon the completion of HMP study enrollment. Variables include additional health history such as dietary habits, breastfeeding, birthing history, delivery method, and if the subject failed any initial screenings prior to enrollment.

#### See Also

attach\_dbGaP

## **Examples**

head(dictionary)

HMP16SData

16S rRNA sequencing data from the Human Microbiome Project

## Description

HMP16SData is a Bioconductor ExperimentData package of the Human Microbiome Project (HMP) 16S rRNA sequencing data for variable regions 1–3 and 3–5. Raw data files are provided in the package as downloaded from the HMP Data Analysis and Coordination Center. Processed data is provided as SummarizedExperiment-class objects via ExperimentHub.

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kable\_one

Produce a summary HTML table of key demographic variables

#### **Description**

Sometimes it is desirable to produce a summary of key demographic variables for presentation. The table\_one and kable\_one methods are a quick way to do so – they not only summarize key demographic variables from SummarizedExperiment-class object(s) in the HMP16SData package but remove abbreviations and underscores in column and variable names that might otherwise be ambigious. The table\_one method returns a *tidy* (i.e. one sample observation per line) data.frame object or a named list of *tidy* data.frame objects. The kable\_one method can then be used to produce a publication-ready HTML table that could, for example, be pasted into a word processor.

#### Usage

```
kable_one(x, significant_figures = 2)
```

#### Arguments

The number of significant figures to be used for decimals in the HTML table; if no value is specified, the default is 2

#### Value

A summary HTML table of key demographic variables

#### See Also

```
table_one
```

#### **Examples**

```
V13() %>%
table_one() %>%
kable_one()
```

table\_one

Produce a summary data.frame of key demographic variables

#### **Description**

Sometimes it is desirable to produce a summary of key demographic variables for presentation. The table\_one and kable\_one methods are a quick way to do so – they not only summarize key demographic variables from SummarizedExperiment-class object(s) in the HMP16SData package but remove abbreviations and underscores in column and variable names that might otherwise be ambigious. The table\_one method returns a *tidy* (i.e. one sample observation per line) data.frame object or a named list of *tidy* data.frame objects. The kable\_one method can then be used to produce a publication-ready HTML table that could, for example, be pasted into a word processor.

#### **Usage**

```
table_one(x, VISITNO = TRUE, SEX = TRUE, RUN_CENTER = TRUE,
    HMP_BODY_SITE = TRUE, HMP_BODY_SUBSITE = TRUE)
```

#### Arguments

 $x \hspace{1cm} A \hspace{1cm} \textbf{SummarizedExperiment-class} \hspace{1cm} \textbf{object} \hspace{1cm} \textbf{or} \hspace{1cm} \textbf{a} \hspace{1cm} \textbf{named} \hspace{1cm} \textbf{list} \hspace{1cm} \textbf{of} \hspace{1cm} \textbf{SummarizedExperiment-class} \\$ 

objects from the HMP16SData package

VISITNO logical; if FALSE, the VISITNO column(s) of SummarizedExperiment colData

will not be summarized

SEX logical; if FALSE, the SEX column(s) of SummarizedExperiment colData will

not be summarized

RUN\_CENTER logical; if FALSE, the RUN\_CENTER column(s) of SummarizedExperiment colData

will not be summarized

HMP\_BODY\_SITE logical; if FALSE, the HMP\_BODY\_SITE column(s) of SummarizedExperiment

colData will not be summarized

HMP\_BODY\_SUBSITE

logical; if FALSE, the HMP\_BODY\_SUBSITE column(s) of SummarizedExperiment

colData will not be summarized

#### Value

A data.frame object or a named list of data.frame objects

#### See Also

kable\_one

#### **Examples**

```
V13() %>%
table_one()
```

V13

HMP 16S rRNA sequencing data for variable regions 1–3

#### **Description**

The NIH Human Microbiome Project (HMP) was a longitudinal study conducted from 2007 to 2012 across four institutions (Baylor College of Medicine, the Broad Institute, the J. Craig Venter Institute, and Washington University) of healthy adults aged 18 to 40 that produced a comprehensive reference for the composition, diversity, and variation of the healthy human microbiome. This SummarizedExperiment-class object represents 16S rRNA sequencing data for variable regions 1–3 that was performed on samples collected at five major body sites – available participant metadata as well as phylogenetic trees are included.

#### Usage

```
V13(metadata = FALSE)
```

#### **Arguments**

metadata

logical; if TRUE only the metadata is downloaded, rather than the entire resource

#### **Format**

A SummarizedExperiment-class object with 43,140 features and 2,898 samples:

#### colData:

**RSID** a random subject identifier

**VISITNO** visit number, between 1 and 3

**SEX** sex, female or male

**RUN\_CENTER** center where sample sequencing took place: Baylor College of Medicine (BCM), the Broad Institute (BI), the J. Craig Venter Institute (JCVI), or the Genome Sequencing Center at Washington University (WUGC)

HMP\_BODY\_SITE body site where the sample was collected

HMP\_BODY\_SUBSITE body subsite where the sample was collected

**SRS\_SAMPLE\_ID** a sample identifier to be used when comparing 16S rRNA samples to whole metagenome shotgun (WMS) samples

#### rowData:

CONSENSUS\_LINEAGE the most detailed lineage description shared by the sequences within an OTU

SUPERKINGDOM superkingdom taxonomy, assumed to be Bacteria

PHYLUM phylum taxonomy parsed from CONSENSUS\_LINEAGE

CLASS calss taxonomy parsed from CONSENSUS\_LINEAGE

**ORDER** order taxonomy parsed from CONSENSUS\_LINEAGE

FAMILY family taxonomy parsed from CONSENSUS\_LINEAGE

GENUS genus taxonomy parsed from CONSENSUS\_LINEAGE

#### Value

A SummarizedExperiment-class object

#### Note

The "PSN" identifiers were used as the colnames of the SummarizedExperiment-class object, see source for additional information.

#### Source

The following source information is derived from the HMP Data Analysis and Coordination Center:

Following a July 2010 16S data freeze, data was downloaded from NCBI SRA projects SRP002395: Human Microbiome Project 16S rRNA Clinical Production Phase I, and SRP002012: Human Microbiome Project 454 Clinical Production Pilot. This dataset corresponds to over 5,700 samples and over 10,000 sequence preps. 16S variable region 3–5 (V35) was sequenced for the entire set of samples, and variable region 1–3 (V13) for a subset of samples.

The QIIME (Quantitative Insights Into Microbial Ecology) software package was used to process HMP 16S data using an OTU-binning strategy to which taxonomic classification is added.

Raw 16S sequence and metadata, available through <a href="https://tinyurl.com/y7ev836z">https://tinyurl.com/y7ev836z</a>, were demultiplexed using QIIME. OTU picking was performed for the V1–3 and V3–5 region sequences

using OTUPipe, which includes error correction, chimera checking through UCHIME, and clustering via UCLUST, and postprocessing by picking the optimal representative sequence centroid. Taxonomy was assigned using the RDP classifier version 2.2.

The resulting OTU tables were checked for mislabeling and contamination, as described in the SOP available through <a href="https://tinyurl.com/y7ev836z">https://tinyurl.com/y7ev836z</a>. Alpha and beta diversity for each sample and Procrustes analysis were established using QIIME with default parameters.

All QIIME output files are available through https://tinyurl.com/y7ev836z, for both the V1–3 and V3–5 variable regions, as well as Procrustes summary data. SOPs and custom scripts are also available through https://tinyurl.com/y7ev836z.

If you're interested in joint analysis of 16S and shotgun metagenomic datasets from the HMP, pairing up data from the same microbiome samples can initially seem tricky. The HMP Sample Flow Schematic indicates how these sample IDs are related experimentally, and provides tables joining 16S dataset "SN" and "PSN" identifiers with metagenomic dataset "SRS" identifiers.

Four files were used to construct this SummarizedExperiment-class object.

OTU table file with PSN identifiers: https://tinyurl.com/y74gqpho
Subject metadata files with PSN identifiers: https://tinyurl.com/y8adlfso
Subject metadata files with SRS identifiers: https://tinyurl.com/ybmn7q8m
Representative sequence phylogenetic trees: https://tinyurl.com/ybp8mzgj

#### See Also

V35

#### **Examples**

V13()

V35

HMP 16S rRNA sequencing data for variable regions 3–5

## **Description**

The NIH Human Microbiome Project (HMP) was a longitudinal study conducted from 2007 to 2012 across four institutions (Baylor College of Medicine, the Broad Institute, the J. Craig Venter Institute, and Washington University) of healthy adults aged 18 to 40 that produced a comprehensive reference for the composition, diversity, and variation of the healthy human microbiome. This SummarizedExperiment-class object represents 16S rRNA sequencing data for variable regions 3–5 that was performed on samples collected at five major body sites – available participant metadata as well as phylogenetic trees are included.

#### Usage

```
V35(metadata = FALSE)
```

#### **Arguments**

metadata

logical; if TRUE only the metadata is downloaded, rather than the entire resource

#### **Format**

A SummarizedExperiment with 45,383 features and 4,743 samples:

#### colData:

**RSID** a random subject identifier

**VISITNO** visit number, between 1 and 3

SEX sex, female or male

**RUN\_CENTER** center where sample sequencing took place: Baylor College of Medicine (BCM), the Broad Institute (BI), the J. Craig Venter Institute (JCVI), or the Genome Sequencing Center at Washington University (WUGC)

HMP\_BODY\_SITE body site where the sample was collected

HMP\_BODY\_SUBSITE body subsite where the sample was collected

**SRS\_SAMPLE\_ID** a sample identifier to be used when comparing 16S rRNA samples to whole metagenome shotgun (WMS) samples

#### rowData:

**CONSENSUS\_LINEAGE** the most detailed lineage description shared by the sequences within an OTU

**SUPERKINGDOM** superkingdom taxonomy, assumed to be Bacteria

PHYLUM phylum taxonomy parsed from CONSENSUS\_LINEAGE

**CLASS** calss taxonomy parsed from CONSENSUS\_LINEAGE

**ORDER** order taxonomy parsed from CONSENSUS\_LINEAGE

FAMILY family taxonomy parsed from CONSENSUS\_LINEAGE

**GENUS** genus taxonomy parsed from CONSENSUS\_LINEAGE

#### Value

A SummarizedExperiment object

#### Note

The "PSN" identifiers were used as the colnames of the SummarizedExperiment object, see source for additional information.

#### **Source**

The following source information is derived from the HMP Data Analysis and Coordination Center:

Following a July 2010 16S data freeze, data was downloaded from NCBI SRA projects SRP002395: Human Microbiome Project 16S rRNA Clinical Production Phase I, and SRP002012: Human Microbiome Project 454 Clinical Production Pilot. This dataset corresponds to over 5,700 samples and over 10,000 sequence preps. 16S variable region 3–5 (V35) was sequenced for the entire set of samples, and variable region 1–3 (V13) for a subset of samples.

The QIIME (Quantitative Insights Into Microbial Ecology) software package was used to process HMP 16S data using an OTU-binning strategy to which taxonomic classification is added.

Raw 16S sequence and metadata, available through <a href="https://tinyurl.com/y7ev836z">https://tinyurl.com/y7ev836z</a>, were demultiplexed using QIIME. OTU picking was performed for the V1–3 and V3–5 region sequences using OTUPipe, which includes error correction, chimera checking through UCHIME, and clustering via UCLUST, and postprocessing by picking the optimal representative sequence centroid. Taxonomy was assigned using the RDP classifier version 2.2.

The resulting OTU tables were checked for mislabeling and contamination, as described in the SOP available through <a href="https://tinyurl.com/y7ev836z">https://tinyurl.com/y7ev836z</a>. Alpha and beta diversity for each sample and Procrustes analysis were established using QIIME with default parameters.

All QIIME output files are available through https://tinyurl.com/y7ev836z, for both the V1–3 and V3–5 variable regions, as well as Procrustes summary data. SOPs and custom scripts are also available through https://tinyurl.com/y7ev836z.

If you're interested in joint analysis of 16S and shotgun metagenomic datasets from the HMP, pairing up data from the same microbiome samples can initially seem tricky. The HMP Sample Flow Schematic indicates how these sample IDs are related experimentally, and provides tables joining 16S dataset "SN" and "PSN" identifiers with metagenomic dataset "SRS" identifiers.

Four files were used to construct this SummarizedExperiment-class object.

OTU table file with PSN identifiers: https://tinyurl.com/y9rbpj17

Subject metadata files with PSN identifiers: https://tinyurl.com/yaz35f22 Subject metadata files with SRS identifiers: https://tinyurl.com/y9xjqm29 Representative sequence phylogenetic trees: https://tinyurl.com/y9exxlgr

#### See Also

V13

#### **Examples**

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