# Package 'MIC'

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Title Analysis of Antimicrobial Minimum Inhibitory Concentration Data

Version 1.1.0

Description Analyse, plot, and tabulate antimicrobial minimum inhibitory concentration (MIC) data. Validate the results of an MIC experiment by comparing observed MIC values to a gold standard assay, in line with standards from the International Organization for Standardization (2021) <https: //www.iso.org/standard/79377.html>. Perform MIC prediction from whole genome sequence data stored in the Pathosystems Resource Integration Center (2013) <doi:10.1093/nar/gkt1099> database or locally.

**License** GPL (>= 3)

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as.sir\_vectorised Convert MIC or Disk Diffusion to SIR, vectorised over antimicrobials

## Description

The AMR::as.sir function is not vectorised over antimicrobials. This function provides vectorisation over antimicrobials. Due to the overhead of running AMR::as.sir, this function tries to be efficient by only running AMR::as.sir as little as necessary.

## Usage

as.sir\_vectorised(mic, mo, ab, accept\_ecoff = FALSE, ...)

## Arguments

mic	vector of MIC values
mo	vector of microorganism names
ab	vector of antibiotic names
accept_ecoff	if TRUE, ECOFFs will be used when no clinical breakpoints are available
	additional arguments that are passed to AMR::as.sir

#### Value

S3 sir values

```
mic <- c("<0.25", "8", "64", ">64")
mo <- c("B_ESCHR_COLI", "B_ESCHR_COLI", "B_ESCHR_COLI", "B_ESCHR_COLI")
ab <- c("AMK", "AMK", "AMK")
as.sir_vectorised(mic, mo, ab)
# using different microorganisms and antibiotics
mic <- c("<0.25", "8", "64", ">64")
mo <- c("B_ESCHR_COLI", "B_ESCHR_COLI", "B_PROTS_MRBL", "B_PROTS_MRBL")
ab <- c("AMK", "AMK", "CIP", "CIP")
as.sir_vectorised(mic, mo, ab)
```

bias

#### Description

Calculate the bias between two AMR::mic vectors. The bias is calculated as the percentage of test MICs that are above the gold standard MICs minus the percentage of test MICs that are below the gold standard MICs.

#### Usage

```
bias(gold_standard, test)
```

#### Arguments

gold\_standard AMR::mic vector test AMR::mic vector

## Value

numeric value

#### References

International Organization for Standardization. ISO 20776-2:2021 Available from: https://www.iso.org/standard/79377.html

#### Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
bias(gold_standard, test)</pre>
```

clean\_raw\_mic Clean up raw MIC for use as a feature

#### Description

Removes leading "=" which can sometimes be present in raw MIC results. Also converts cotrimoxazole to trimethprim component only.

#### Usage

clean\_raw\_mic(mic)

#### Arguments

mic character containing MIC/s

## combined\_file\_system

## Value

character of clean MIC/s

## Examples

```
clean_raw_mic(c("==>64","0.25/8.0"))
```

combined\_file\_system Combine train and test filesystem into single folder

#### Description

This function reorganises files that have been split into train and test directories using train\_test\_filesystem() back into a single directory. This is a convenience function to reverse the effects of train\_test\_filesystem().

## Usage

```
combined_file_system(
   path_to_folders,
   file_ext,
   train_folder = "train",
   test_folder = "test",
   overwrite = FALSE
)
```

## Arguments

path\_to\_folders

	path containing test and train folders; files will be moved here
file_ext	file extension to filter
train_folder	train folder subdirectory name
test_folder	test folder subdirectory name
overwrite	force overwrite of files that already exist

## Value

Logical vector, indicated success or failure for each file

```
set.seed(123)
# create 10 random DNA files
tmp_dir <- tempdir()
# remove any existing .fna files
file.remove(
    list.files(tmp_dir, pattern = "*.fna", full.names = TRUE)
)</pre>
```

compare\_mic

Compare and validate MIC values

#### Description

This function compares an vector of MIC values to another. Generally, this is in the context of a validation experiment – an investigational assay or method (the "test") is compared to a gold standard. The rules used by this function are in line with "ISO 20776-2:2021 Part 2: Evaluation of performance of antimicrobial susceptibility test devices against reference broth micro-dilution."

There are two levels of detail that are provided. If only the MIC values are provided, the function will look for essential agreement between the two sets of MIC. If the organism and antibiotic arguments are provided, the function will also calculate the categorical agreement using EUCAST breakpoints (or, if breakpoint not available and accept\_ecoff = TRUE, ECOFFs).

The function returns a special dataframe of results, which is also an mic\_validation object. This object can be summarised using summary() for summary metrics, plotted using plot() for an essential agreement confusion matrix, and tabulated using table().

#### Usage

```
compare_mic(
 gold_standard,
 test,
 ab = NULL,
 mo = NULL,
 accept_ecoff = FALSE,
 simplify = TRUE,
 ea_mode = "categorical",
 tolerate_censoring = "gold_standard",
 tolerate_matched_censoring = "both",
 ....
)
```

#### compare\_mic

#### Arguments

gold_standard	vector of MICs to compare against.
test	vector of MICs that are under investigation
ab	character vector (same length as MIC) of antibiotic names (optional)
mo	character vector (same length as MIC) of microorganism names (optional)
accept_ecoff	if TRUE, ECOFFs will be used when no clinical breakpoints are available
simplify	if TRUE, MIC values will be coerced into the closest halving dilution (e.g., 0.55 will be converted to 0.5)
ea_mode	"categorical" or "numeric", see essential_agreement
tolerate_censo	ring "strict", "gold_standard", "test", or "both" - how to handle censored data (see es- sential_agreement for details). Generally, this should be left as "gold_standard" since this setting "tolerates" a test that has higher granularity (i.e., less censor- ing) than the gold standard. Setting to "test" or "both" should be used with cau- tion but may be appropriate in some cases where the test also produces censored results.
tolerate_match	ed_censoring "strict", "gold_standard", "test", or "both" - how to handle situations where one of the values is censored, but both values match (e.g., gold_standard = ">2", test = "2"). Generally, this should be left as "both", since these values are considered to be in essential agreement. For more details, see essential_agreement. additional arguments to be passed to AMR::as.sir

## Value

S3 mic\_validation object

```
# Just using MIC values only
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
summary(val)
# Using MIC values and antibiotic and organism names
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
ab <- c("AMK", "AMK", "AMK", "AMK")
mo <- c("B_ESCHR_COLI", "B_ESCHR_COLI", "B_ESCHR_COLI")</pre>
```

```
val <- compare_mic(gold_standard, test, ab, mo)</pre>
```

```
"error" %in% names(val) # val now has categorical agreement
```

```
compare_sir
```

#### Description

Compare two AMR::sir vectors and generate a categorical agreement vector with the following levels: M (major error), vM (very major error), m (minor error). The error definitions are:

- 1. Major error (M): The test result is resistant (R) when the gold standard is susceptible (S).
- 2. vM (very major error): The test result is susceptible (S) when the gold standard is resistant (R).
- 3. Minor error (m): The test result is intermediate (I) when the gold standard is susceptible (S) or resistant (R), or vice versa.

#### Usage

compare\_sir(gold\_standard, test)

## Arguments

gold_standard	Susceptibility results in AMR::sir format
test	Susceptibility results in AMR::sir format

#### Value

factor vector with the following levels: M, vM, m.

#### Examples

```
gold_standard <- c("S", "R", "I", "I")
gold_standard <- AMR::as.sir(gold_standard)
test <- c("S", "I", "R", "R")
test <- AMR::as.sir(test)
compare_sir(gold_standard, test)</pre>
```

#### Description

Download PATRIC database

#### Usage

```
download_patric_db(save_path, ftp_path = patric_ftp_path, overwrite = FALSE)
```

#### Arguments

save_path	Save path (should be .txt)
ftp_path	PATRIC database FTP path to download
overwrite	Force overwrite

## Value

TRUE if successful, FALSE if failure.

## Examples

download\_patric\_db(tempfile())

droplevels.mic\_validation Droplevels for MIC validation object

## Description

Quite often, MIC values are being compared across methods with different levels of granularity. For example, the true MIC may be measured across a higher range of values than the test method. This means that there may be MIC levels that don't provide much additional information (since they are only present in one of the methods). This function removes these unnecessary levels at both ranges of the MIC values.

This function ensure that the changes do not "change" the essential agreement interpretation. This can be suppressed using safe = FALSE, however this is probably not desired behaviour.

## Usage

```
## S3 method for class 'mic_validation'
droplevels(x, safe = TRUE, ...)
```

## Arguments

х	mic_validation object
safe	ensure that essential agreement is not changed after dropping levels
	additional arguments

## Value

mic\_validation object

ecoffs

#### Examples

```
gold_standard <- c("<0.25", "0.25", "0.5", "1", "2", "1", "0.5")
test <- c("0.004", "0.08", "<0.25", "0.5", "1", "0.5", "0.5")
val <- compare_mic(gold_standard, test)
droplevels(val)</pre>
```

ecoffs

ECOFF data

## Description

A dataset containing the epidemiological cut-off values (ECOFFs) for different antibiotics and microorganisms. Currently, only the ECOFF values for *Escherichia coli* are included.

#### Usage

ecoffs

## Format

ecoffs:

A data frame with 85 rows and 25 columns:

organism Microorganism code in AMR::mo format

antibiotic Antibiotic code in AMR::ab format

0.002:512 Counts of isolates in each concentration "bin"

**Distributions** see EUCAST documentation below

**Observations** Number of observations

(T)ECOFF see EUCAST documentation below

Confidence interval see EUCAST documentation below

#### Source

#### EUCAST https://www.eucast.org/mic\_and\_zone\_distributions\_and\_ecoffs

These data have (or this document, presentation or video has) been produced in part under ECDC service contracts and made available by EUCAST at no cost to the user and can be accessed on the EUCAST website www.eucast.org. The views and opinions expressed are those of EUCAST at a given point in time. EUCAST recommendations are frequently updated and the latest versions are available at www.eucast.org.

essential\_agreement Essential agreement for MIC validation

#### Description

Essential agreement calculation for comparing two MIC vectors.

#### Usage

```
essential_agreement(
    x,
    y,
    coerce_mic = TRUE,
    tolerate_censoring = "strict",
    tolerate_matched_censoring = "both",
    mode = "categorical"
)
```

## Arguments

х	AMR::mic or coercible
У	AMR::mic or coercible
coerce_mic	convert to AMR::mic
tolerate_censor	ing
	"strict", "x", "y", or "both" - whether to tolerate censoring in x, y, or both. See
	details.
<pre>tolerate_matche</pre>	d_censoring
	"strict", "x", "y", or "both" - how to handle situations where one of the values is censored, but both values match (e.g., $x = ">2"$ , $y = "2"$ ). For most situations, this is considered essential agreement. so should be left as "both".
mode	"categorical" or "numeric", see details

#### Details

Essential agreement is a central concept in the comparison of two sets of MIC values. It is most often used when validating a new method against a gold standard. This function reliably performs essential agreement in line with ISO 20776-2:2021. The function can be used in two modes: categorical and numeric. In categorical mode, the function will use traditional MIC concentrations to determine the MIC (therefore it will use force\_mic() to convert both x and y to a clean MIC – see force\_mic). In numeric mode, the function will compare the ratio of the two MICs, after removing censoring (values that are ">" and "<" are multiplied and divided by 2, respectively — see mic\_uncensor). In most cases, categorical mode provides more reliable results. Values within +/- 1 dilutions are considered to be in essential agreement.

The tolerate\_censoring argument controls how the function handles censored data. If set to "strict", the function will return NA for any pair of values that are both censored (and not equal). If set to "x" or "y", the function will allow one of the values to be censored and will compare the uncensored

value to the other value. When set to "both", the function will allow one of the values to be censored. If using "both" and both values are censored, the function will attempt to determine essential agreement based on the ratio of the two values, but a warning will be raised.

## Value

logical vector

## References

International Organization for Standardization. ISO 20776-2:2021 Available from: https://www.iso.org/standard/79377.html

#### Examples

```
x <- AMR::as.mic(c("<0.25", "8", "64", ">64"))
y <- AMR::as.mic(c("<0.25", "2", "16", "64"))
essential_agreement(x, y)
# TRUE FALSE FALSE TRUE
# examples using tolerate_censoring
x <- AMR::as.mic("<4")
y <- AMR::as.mic("0.25")
essential_agreement(x, y, tolerate_censoring = "x") # TRUE
essential_agreement(x, y, tolerate_censoring = "y") # FALSE
essential_agreement(x, y, tolerate_censoring = "both") # TRUE (same as "x")
# strict returns FALSE as it wants the censoring cut-offs to be close
essential_agreement(x, y, tolerate_censoring = "strict")
```

example\_mics Example MIC data

#### Description

Example minimum inhibitory concentration validation data for three antimicrobials on Escherichia coli strains. This data is synthetic and generated to give an example of different MIC distribution.

#### Usage

example\_mics

#### Format

example\_mics:
A data frame with 300 rows and 4 columns:
gs Gold standard MICs
test Test MICs
mo Microorganism code in AMR::mo format
ab Antibiotic code in AMR::ab format

## fill\_dilution\_levels

## Source

Synthetic data

fill\_dilution\_levels Fill MIC dilution levels

#### Description

Fill MIC dilution levels

## Usage

```
fill_dilution_levels(x, cap_upper = TRUE, cap_lower = TRUE, as.mic = TRUE)
```

## Arguments

х	MIC vector
cap_upper	If True, will the top level will be the highest MIC dilution in x
cap_lower	If True, will the bottom level will be the lowest MIC dilution in x
as.mic	By default, returns an ordered factor. Set as.mic = TRUE to return as AMR::mic

## Value

ordered factor (or AMR::mic if as.mic = TRUE)

## Examples

```
# use in combination with droplevels to clean up levels:
x <- AMR::as.mic(c("<0.25", "8", "64", ">64"))
x <- droplevels(x)
fill_dilution_levels(x)
```

force\_mic

Force MIC-like into MIC-compatible format

#### Description

Convert a value that is "almost" an MIC into a valid MIC value.

#### Usage

```
force_mic(
  value,
  levels_from_AMR = FALSE,
  max_conc = 512,
  min_conc = 0.002,
  method = "closest",
  prefer = "max"
)
```

#### Arguments

value	vector of MIC-like values (numeric or character)		
levels_from_AMM	levels_from_AMR		
	conform to AMR::as.mic levels		
max_conc	maximum concentration to force to		
<pre>min_conc</pre>	minimum concentration to force to		
method	method to use when forcing MICs (closest or round_up)		
prefer	where value is in between MIC (e.g., 24mg/L) chose the higher MIC ("max") or lower MIC ("min"); only applies to method = "closest"		

## Details

Some experimental or analytical conditions measure MIC (or surrogate) in a way that does not fully conform to traditional MIC levels (i.e., concentrations). This function allows these values to be coerced into an MIC value that is compatible with the AMR::mic class. When using method = "closest", the function will choose the closest MIC value to the input value (e.g., 2.45 will be coerced to 2). When using method = "round up", the function will round up to the next highest MIC value (e.g., 2.45 will be coerced to 4). "Round up" is technically the correct approach if the input value was generated from an experiment that censored between concentrations (e.g., broth or agar dilution). However, "closest" may be more appropriate in some cases.

#### Value

AMR::as.mic compatible character

## Examples

```
force_mic(c("2.32", "<4.12", ">1.01"))
```

genomes\_to\_kmer\_libsvm

Convert genomes to kmers in libsvm format

#### Description

Raw genome data (pre- or post-assembly) is usually transformed by k-mer counting prior to machine learning (ML). XGBoost is a popular ML algorithm for this problem, due to its scalability to high dimensional data. This function converts genomes to k-mer counts stored in XGBoost's preferred format, libsvm. Further information on the libsvm format is available at https://xgboost. readthedocs.io/en/stable/tutorials/input\_format.html. Briefly, libsvm is effectively a text file that stores data points as x:y pairs, where x is the feature index, and y is the feature value. Each observation is stored on its own line, with the first column reserved for labels. Labels can be provided later, during data import.

This function converts each individual genome to an individual libsvm text file of k-mer counts (therefore, each .txt file will be 1 line long). This function supports parallel processing using the by setting an appropriate future::plan() (usually future::multisession) — each genome is processed in parallel. To monitor progress, use the progressr package by wrapping the function in with\_progress.

Although XGBoost can load a multiple .txt (libsvm) files by providing the directory as an input, this is generally not recommended as order of import cannot be guaranteed and probably depends on filesystem. Instead, it is recommended that this function is combined with split\_and\_combine\_files() which generates a single .txt file (with the order of observations guaranteed and stored in a .csv file).

#### Usage

```
genomes_to_kmer_libsvm(
   source_dir,
   target_dir,
   k = 3,
   canonical = TRUE,
   squeeze = FALSE,
   ext = ".fna"
)
```

#### Arguments

source_dir	directory containing genomes
target_dir	target directory to store kmers in libsvm format
k	k-mer length
canonical	only count canonical kmers
squeeze	remove non-canonical kmers
ext	file extension to filter

#### Value

TRUE if successful

## See Also

to convert a single genome, use genome\_to\_libsvm()

## Examples

```
set.seed(123)
# create 10 random DNA files
tmp_dir <- tempdir()</pre>
# remove any existing .fna files
file.remove(
list.files(tmp_dir, pattern = "*.fna", full.names = TRUE)
)
for (i in 1:10) {
writeLines(paste0(">", i, "\n", paste0(sample(c("A", "T", "C", "G"),
100, replace = TRUE), collapse = "")), file.path(tmp_dir, paste0(i, ".fna")))
}
tmp_target_dir <- file.path(tmp_dir, "kmers")</pre>
unlink(tmp_target_dir, recursive = TRUE)
# convert genomes to k-mers
future::plan(future::sequential) # use multisession for parallel processing
progressr::with_progress(
  genomes_to_kmer_libsvm(tmp_dir, tmp_target_dir, k = 3)
)
# check the output
list.files(tmp_target_dir)
readLines(list.files(tmp_target_dir, full.names = TRUE)[1])
```

genome\_to\_libsvm Converts a genome to kmers stored in libsvm format on disk

## Description

This function converts a single genome to a libsym file containing kmer counts. The libsym format will be as follows:

label 1:count 2:count 3:count ...

Label is optional and defaults to 0. The kmer counts are indexed by the kmer index, which is the lexicographically sorted index of the kmer. Libsvm is a sparse format.

## genome\_to\_libsvm

## Usage

```
genome_to_libsvm(
    x,
    target_path,
    label = as.character(c("0")),
    k = 3L,
    canonical = TRUE,
    squeeze = FALSE,
    overwrite = FALSE
)
```

## Arguments

х	genome in string format
target_path	path to store libsvm file (.txt)
label	libsvm label
k	kmer length
canonical	only record canonical kmers (i.e., the lexicographically smaller of a kmer and its reverse complement)
squeeze	remove non-canonical kmers
overwrite	overwrite existing file

## Value

boolean indicating success

## See Also

For multiple genomes in a directory, processed in parallel, see genomes\_to\_kmer\_libsvm()

For more details on libsvm format, see https://xgboost.readthedocs.io/en/stable/tutorials/ input\_format.html

```
temp_libsvm_path <- tempfile(fileext = ".txt")
genome_to_libsvm("ATCGCAGT", temp_libsvm_path)
readLines(temp_libsvm_path)</pre>
```

## get\_mic

#### Description

This function helps extract MICs from a database of results. It is compatible with the PATRIC meta data format when used on a tidy\_patric\_db object, created using tidy\_patric\_db().

If more than one MIC is present for a particular observation, the function can return the higher MIC by setting prefer\_high\_mic = TRUE. If prefer\_high\_mic = FALSE, the lower MIC will be returned.

#### Usage

```
get_mic(
    x,
    ids,
    ab_col,
    id_col = NULL,
    as_mic = TRUE,
    prefer_high_mic = TRUE,
    simplify = TRUE
)
```

#### Arguments

х	dataframe containing meta-data
ids	vector of IDs to get meta-data for
ab_col	column name containing MIC results
id_col	column name containing IDs
as_mic	return as AMR::as.mic
prefer_high_mi	c
	where multiple MIC results per ID, prefer the higher MIC
simplify	return as vector of MICs (vs dataframe)

#### Value

vector containing MICs, or dataframe of IDs and MICs

```
df <- data.frame(genome_id = c("a_12", "b_42", "x_21", "x_21", "r_75"),
            gentamicin = c(0.25, 0.125, 32.0, 16.0, "<0.0125"))
get_mic(df,
            ids = c("b_42", "x_21"),
            ab_col = "gentamicin",
            id_col = "genome_id",
            as_mic = FALSE,
```

kmers

```
prefer_high_mic = TRUE,
simplify = TRUE)
```

kmers

#### Generates genome kmers

## Description

Generates genome kmers

## Usage

```
kmers(
    x,
    k = 3L,
    simplify = FALSE,
    canonical = TRUE,
    squeeze = FALSE,
    anchor = TRUE,
    clean_up = TRUE,
    key_as_int = FALSE,
    starting_index = 1L
)
```

## Arguments

х	genome in string format
k	kmer length
simplify	returns a numeric vector of kmer counts, without associated string. This is useful to save memory, but should always be used with anchor = true.
canonical	only record canonical kmers (i.e., the lexicographically smaller of a kmer and its reverse complement)
squeeze	remove non-canonical kmers
anchor	includes unobserved kmers (with counts of 0). This is useful when generating a dense matrix where kmers of different genomes align.
clean_up	only include valid bases (ACTG) in kmer counts (excludes non-coding results such as $N) \end{tabular}$
key_as_int	return kmer index (as "kmer_index") rather than the full kmer string. Useful for index-coded data structures such as libsvm.
starting_index	the starting index, only used if key_as_int = TRUE.

## Value

list of kmer values, either as a list of a single vector (if simplify = TRUE), or as a named list containing "kmer\_string" and "kmer\_value".

## Examples

kmers("ATCGCAGT")

load\_patric\_db Load PATRIC database

## Description

Load PATRIC database

## Usage

load\_patric\_db(x = patric\_ftp\_path)

## Arguments

Х

Character path to local or ftp path (.txt or .rds), or data.frame object.

#### Value

PATRIC database (S3 class 'patric\_db')

## Examples

mic\_censor

#### Description

MIC datasets often arise from different laboratories or experimental conditions. In practice, this means that there can be different levels of censoring (<= and >) within the data. This function can be used to harmonise the dataset to a single level of censoring. The function requires a set of rules that specify the censoring levels (see example).

#### Usage

```
mic_censor(mic, ab = NULL, mo = NULL, rules = NULL, max = Inf, min = -Inf)
```

#### Arguments

mic	MIC (coercible to AMR::as.mic)
ab	antibiotic name (coercible to AMR::as.ab)
mo	microorganism name (coercible to AMR::as.mo)
rules	censor rules - named list of pathogen (in AMR::as.mo code) to antibiotic (in AMR::as.ab code) to censoring rules. The censoring rules should provide a min or max value to censor MICs to. See example for more.
max	maximum concentration to censor to (default = Inf), will override any rules pro- vided
min	minimum concentration to censor to (default = -Inf), will override any rules provided

## Value

censored MIC values (S3 mic class)

#### Examples

```
example_rules <- list("B_ESCHR_COLI" = list(
    "AMK" = list(min = 2, max = 32),
    "CHL" = list(min = 4, max = 64),
    "GEN" = list(min = 1, max = 16),
    "CIP" = list(min = 0.015, max = 4),
    "MEM" = list(min = 2, max = 64),
    "AMX" = list(min = 2, max = 64),
    "FEP" = list(min = 0.5, max = 64),
    "CAZ" = list(min = 1, max = 128),
    "TGC" = list(min = 0.25, max = 1)
    ))</pre>
```

mic\_censor(AMR::as.mic(512),

```
"AMK",
"B_ESCHR_COLI",
example_rules) == AMR::as.mic(">32")
```

mic\_range

Generate dilution series

## Description

Generate dilution series

## Usage

```
mic_range(start = 512, dilutions = Inf, min = 0.002, precise = FALSE)
```

## Arguments

start	starting (highest) concentration
dilutions	number of dilutions
min	minimum (lowest) concentration
precise	force range to be high precision (not usually desired behaviour)

#### Value

Vector of numeric concentrations

## Examples

```
mic_range(128)
mic_range(128, dilutions = 21) # same results
```

## Description

R breakpoint for MIC

## Usage

```
mic_r_breakpoint(mo, ab, accept_ecoff = FALSE, ...)
```

## Arguments

mo	mo name (coerced using AMR::as.mo)
ab	ab name (coerced using AMR::as.ab)
accept_ecoff	if TRUE, ECOFFs will be used when no clinical breakpoints are available
	additional arguments to pass to AMR::as.sir, which is used to calculate the R breakpoint

## Value

MIC value

## Examples

```
mic_r_breakpoint("B_ESCHR_COLI", "AMK")
mic_r_breakpoint("B_ESCHR_COLI", "CHL", accept_ecoff = TRUE)
```

mic\_s\_breakpoint S breakpoint for MIC

## Description

S breakpoint for MIC

## Usage

```
mic_s_breakpoint(mo, ab, accept_ecoff = FALSE, ...)
```

## Arguments

mo	mo name (coerced using AMR::as.mo)
ab	ab name (coerced using AMR::as.ab)
accept_ecoff	if TRUE, ECOFFs will be used when no clinical breakpoints are available
	additional arguments to pass to AMR::as.sir, which is used to calculate the S breakpoint

## Value

MIC value

```
mic_s_breakpoint("B_ESCHR_COLI", "AMK")
mic_s_breakpoint("B_ESCHR_COLI", "CHL", accept_ecoff = TRUE)
```

mic\_uncensor

#### Uncensor MICs

#### Description

Uncensor MICs

## Usage

```
mic_uncensor(
   mic,
   method = "scale",
   scale = 2,
   ab = NULL,
   mo = NULL,
   distros = NULL
)
```

#### Arguments

mic	vector of MICs to uncensor; will be coerced to MIC using AMR::as.mic
method	method to uncensor MICs (scale, simple, or bootstrap)
scale	scalar to multiply or divide MIC by (for method = scale)
ab	antibiotic name (for method = bootstrap)
mo	microorganism name (for method = bootstrap)
distros	dataframe of epidemiological distributions (only used, optionally, for method = bootstrap)

#### Details

Censored MIC data is generally unsuitable for modelling without some conversion of censored data. The default behaviour (method = scale) is to halve MICs under the limit of detection (<=) and double MICs above the limit of detection (>). When used with method = simple, this function effectively just removes the censoring symbols, e.g., <=2 becomes 2, and >64 becomes 64.

The bootstrap method is the more complex of the three available methods. It attempts to use a second (uncensored) MIC distribution to sample values in the censored range. These values are then used to populate and uncensor the MIC data provided as input (mic). The second (uncensored) MIC distribution is ideally provided from similar experimental conditions. Alternatively, epidemiological distributions can be used. These distributions should be provided as a dataframe to the distros argument. The format for this dataframe is inspired by the EUCAST epidemiological distributions, see: https://www.eucast.org/mic\_and\_zone\_distributions\_and\_ecoffs. The dataframe should contain columns for antimicrobial (converted using AMR::as.ab), organism (converted using AMR::as.mo), and MIC concentrations. An example is provided in the 'ecoffs' dataset available with this pacakge. Currently, only Escherichia coli is available in this dataset. Each observation (row) consists of the frequency a particular MIC concentration is observed in the distribution. If such a dataframe is not provided to distros, the function will attempt to use 'ecoffs', but remains limited to E. coli.

## move\_files

#### Value

vector of MICs in AMR::mic format

#### References

https://www.eucast.org/mic\_and\_zone\_distributions\_and\_ecoffs

#### Examples

```
mic_uncensor(c(">64.0", "<0.25", "8.0"), method = "scale", scale = 2)</pre>
```

move\_files

Move or copy files using logical vector

## Description

This is simply a wrapper around file.copy/file.rename that allows for filtering by a logical vector (move\_which). This can replicate the behaviour of a predicate function (see example), and may be easier to read.

#### Usage

```
move_files(source_dir, target_dir, move_which, ext = ".txt", copy = FALSE)
```

## Arguments

source_dir	move from directory
target_dir	move to directory
move_which	logical vector to filter (or use TRUE to move all)
ext	file extension to filter
сору	copy files (rather than move)

## Value

Logical vector, indicating success or failure for each file

```
set.seed(123)
# create 10 random DNA files
tmp_dir <- tempdir()
# remove any existing .fna files
file.remove(
    list.files(tmp_dir, pattern = "*.fna", full.names = TRUE)
)
for (i in 1:10) {
writeLines(paste0(">", i, "\n", paste0(sample(c("A", "T", "C", "G"),
```

plot.mic\_validation Plot MIC validation results

## Description

Plot MIC validation results

#### Usage

```
## S3 method for class 'mic_validation'
plot(
    x,
    match_axes = TRUE,
    add_missing_dilutions = TRUE,
    facet_wrap_ncol = NULL,
    facet_wrap_nrow = NULL,
    ...
)
```

#### Arguments

x	object generated using compare_mic	
match_axes	Same x and y axis	
add_missing_dil	utions	
	Axes will include dilutions that are not	
<pre>facet_wrap_ncol</pre>		
	Facet wrap into n columns by antimicrobial (optional, only available when more	
	than one antimicrobial in validation)	
<pre>facet_wrap_nrow</pre>		
	Facet wrap into n rows by antimicrobial (optional, only available when more than one antimicrobial in validation) represented in the data, based on a series of dilutions generated using mic_range().	
	additional arguments	

print.mic\_validation

#### Value

ggplot object

## Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
plot(val)
# if the validation contains multiple antibiotics, i.e.,
ab <- c("CIP", "CIP", "AMK", "AMK")
val <- compare_mic(gold_standard, test, ab)
# the following will plot all antibiotics in a single plot (pooled results)
plot(val)
# use the faceting arguments to split the plot by antibiotic
plot(val, facet_wrap_ncol = 2)
```

print.mic\_validation Print MIC validation object

#### Description

Print MIC validation object

#### Usage

## S3 method for class 'mic\_validation'
print(x, ...)

## Arguments

Х	mic_validation object
	additional arguments

## Value

character

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
print(val)</pre>
```

print.mic\_validation\_summary

Print MIC validation summary

## Description

Print MIC validation summary

#### Usage

## S3 method for class 'mic\_validation\_summary'
print(x, ...)

## Arguments

х	mic_validation_summary object
•••	additional arguments

## Value

character

## Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
print(summary(val))</pre>
```

pull\_PATRIC\_genomes Automated download of genomes from PATRIC database

## Description

Automated download of genomes from PATRIC database

## Usage

```
pull_PATRIC_genomes(
    output_directory,
    taxonomic_name = NULL,
    database = patric_ftp_path,
    filter = "MIC",
    ab = NULL,
    n_genomes = 0
)
```

#### qc\_in\_range

#### Arguments

output_directory	
	local directory to save to
taxonomic_name	character of taxonomic bacterial name to download
database	local or ftp path to PATRIC database, or loaded database using load_patric_db()
filter	"MIC" or "disk" or "all" phenotypes
ab	antibiotic(s) of interest, provided as a character vector of antibiotic names/codes, or ideally, as AMR::ab classes, created using AMR::as.ab (default = all)
n_genomes	number of genomes $(0 = all)$

## Value

The number of failed downloads (i.e., 0 if all attempted downloads were successful).

## Examples

qc\_in\_range

Check that MIC is within QC range

#### Description

Check whether MIC values are within acceptable range for quality control (QC). Every MIC experiment should include a control strain with a known MIC. The results of the experiment are only valid if the control strain MIC falls within the acceptable range. This function checks whether an MIC result is within the acceptable range given: 1) a control strain (usually identified as an ATCC or NCTC number), 2) an antibiotic name, and 3) a guideline (EUCAST or CLSI). The acceptable range is defined by 'QC\_table', which is a dataset which is loaded with this package.

The source of the QC values is the WHONET QC Ranges and Targets available from the 'Antimicrobial Resistance Test Interpretation Engine' (AMRIE) repository: https://github.com/AClark-WHONET/AMRIE

## Usage

```
qc_in_range(
   measurement,
   strain,
   ab,
   ignore_na = TRUE,
   guideline = "EUCAST",
   year = "2023"
)
```

#### Arguments

measurement	measured QC MIC
strain	control strain identifier (usually ATCC)
ab	antibiotic name (will be coerced to AMR::as.ab)
ignore_na	ignores NA (returns TRUE)
guideline	Guideline to use (EUCAST or CLSI)
year	Guideline year (version)

#### Value

logical vector

## References

O'Brien TF, Stelling JM. WHONET: An Information System for Monitoring Antimicrobial Resistance. Emerg Infect Dis. 1995 Jun;1(2):66–66.

#### Examples

```
qc_in_range(AMR::as.mic(0.5), 25922, "GEN") == TRUE
qc_in_range(AMR::as.mic(8.0), 25922, "GEN") == FALSE
```

qc\_on\_target

Check that QC measurement is at the required target [Experimental]

#### Description

MIC experiments should include a control strain with a known MIC. The MIC result for the control strain should be a particular target MIC. This function checks whether the target MIC was achieved given: 1) a control strain (usually identified as an ATCC or NCTC number), 2) an antibiotic name, and 3) a guideline (EUCAST or CLSI).

Since QC target values are currently not publicly available in an easy to use format, this function takes a pragmatic approach – for most antibiotics and QC strains, the target is assumed to be the midpoint of the acceptable range. This approximation is not necessarily equal to the QC target reported by guideline setting bodies such as EUCAST. Therefore, this function is considered experimental and should be used with caution.

This function can be used alongnside qc\_in\_range(), which checks whether the MIC is within the acceptable range.

The source of the QC values is the WHONET QC Ranges and Targets available from the 'Antimicrobial Resistance Test Interpretation Engine' (AMRIE) repository: https://github.com/AClark-WHONET/AMRIE replace\_multiple\_slashes

## Usage

```
qc_on_target(
   measurement,
   strain,
   ab,
   ignore_na = TRUE,
   guideline = "EUCAST",
   year = "2023"
)
```

## Arguments

measurement	measured QC MIC
strain	control strain identifier (usually ATCC)
ab	antibiotic name (will be coerced to AMR::as.ab)
ignore_na	ignores NA (returns TRUE)
guideline	Guideline to use (EUCAST or CLSI)
year	Guideline year (version)

## Value

logical vector

#### References

O'Brien TF, Stelling JM. WHONET: An Information System for Monitoring Antimicrobial Resistance. Emerg Infect Dis. 1995 Jun;1(2):66–66.

## Examples

qc\_on\_target(AMR::as.mic(0.5), 25922, "GEN") == TRUE

replace\_multiple\_slashes

Removes multiple slashes in a path or url

## Description

Removes multiple slashes in a path or url

## Usage

replace\_multiple\_slashes(path)

## Arguments

path character vector

## Value

character vector of paths without duplicate slashes

reverse\_complement Reverse complement of DNA string

## Description

Reverse complement of DNA string

#### Usage

reverse\_complement(dna)

#### Arguments

dna DNA string

#### Value

reverse complement of DNA string

## Examples

```
reverse_complement("ATCG")
```

split\_and\_combine\_files

Create test train files from a number of files

## Description

This function combines files into a train and test set, stored on disk. It can be used in combination with genomes\_to\_kmer\_libsvm() to create a dataset that can be loaded into XGBoost (either by first creating an xgboost::DMatrix, or by using the data argument in xgboost::xgb.train() or xgboost::xgb.cv()). The following three files will be created:

- 1. train.txt the training data
- 2. test.txt the testing data (if split < 1)
- 3. names.csv a csv file containing the original filenames and their corresponding type (train or test)

The function will check if the data is already in the appropriate format and will not overwrite unless forced using the overwrite argument.

By providing 1.0 to the split argument, the function can be used to combine files without a train-test split. In this case, all the files will be classed as 'train', and there will be no 'test' data. This is useful if one wants to perform cross-validation using xgboost::xgb.cv() or MIC::xgb.cv.lowmem(). It is also possible to combine all data into train and then perform splitting after loading into an xgboost::DMatrix, using xgboost::slice().

Usage

```
split_and_combine_files(
   path_to_files,
   file_ext = ".txt",
   split = 0.8,
   train_target_path = NULL,
   test_target_path = NULL,
   names_backup = NULL,
   shuffle = TRUE,
   overwrite = FALSE
)
```

## Arguments

path_to_files	path containing files or vector of filepaths	
file_ext	file extension to filter	
split	train-test split	
train_target_pa	ath	
	name of train file to save as (by default, will be train.txt in the path_to_files directory)	
test_target_path		
	name of test file to save as (by default, will be test.txt in the path_to_files directory)	
names_backup	name of file to save backup of filename metadata (by default, will be names.csv in the path_to_files directory)	
shuffle	randomise prior to splitting	
overwrite	overwrite target files	

## Value

named list of paths to created train/test files, original filenames

```
set.seed(123)
# create 10 random libsvm files
tmp_dir <- tempdir()
# remove any existing .txt files</pre>
```

```
file.remove(
list.files(tmp_dir, pattern = "*.txt", full.names = TRUE)
)
for (i in 1:10) {
 # each line is K: V
 writeLines(paste0(i, ": ", paste0(sample(1:100, 10, replace = TRUE),
 collapse = " ")), file.path(tmp_dir, paste0(i, ".txt")))
 }
 # split files into train and test directories
 paths <- split_and_combine_files(</pre>
  tmp_dir,
  file_ext = "txt",
  split = 0.8,
  train_target_path = file.path(tmp_dir, "train.txt"),
  test_target_path = file.path(tmp_dir, "test.txt"),
  names_backup = file.path(tmp_dir, "names.csv"),
  overwrite = TRUE)
 readLines(paths[["train"]])
```

squeezed\_index\_to\_str Get str conversion of squeezed kmer using index

## Description

Get str conversion of squeezed kmer using index

#### Usage

squeezed\_index\_to\_str(x, k, starting\_index = 1L)

#### Arguments

x	integer vector of kmer indices
k	kmer length

starting\_index starting index (libsvm is usually indexed starting at 1)

## Value

vector of squeezed kmer strings

## Examples

squeezed\_index\_to\_str(2, k = 3)

squeezed\_mers

#### Description

Generates all permutations of squeezed kmers

#### Usage

 $squeezed_mers(k = 3L)$ 

## Arguments k

kmer length

#### Value

vector of squeezed kmers

#### Examples

squeezed\_mers(3)

standardise\_mic Standardise MIC to control strain [Experimental]

#### Description

MIC experiments are generally quality-controlled by including a control strain with a known MIC. The MIC result for the control strain should be a particular target MIC, or at least within an acceptable range. This function standardises a measured MIC to the target MIC given: 1) a control strain (usually identified as an ATCC or NCTC number), 2) an antibiotic name, and 3) a guideline (EUCAST or CLSI). The definition of standardisation in this context is to adjust the measured MIC based on the QC MIC. This is based on the following principles and assumption:

- 1. A measured MIC is composed of two components: the true MIC and a measurement error. The measurement error is considered to be inevitable when measuring MICs, and is likely to be further composed of variability in laboratory conditions and operator interpretation.
- 2. It is assumed that the MIC of the control strain in the experiment has also been affected by this error.

The standardisation applied by this function uses the measured QC strain MIC as a reference point, and scales the rest of the MICs to this reference. In general, this means that the MICs are doubled or halved, depending on the result of the QC MIC. A worked example is provided below and illustrates the transformation that this function applies.

There is no current evidence base for this approach, therefore, this function is considered experimental and should be used with caution.

## Usage

```
standardise_mic(
   test_measurement,
   qc_measurement,
   strain,
   ab,
   prefer_upper = FALSE,
   ignore_na = TRUE,
   guideline = "EUCAST",
   year = "2023",
   force = TRUE
)
```

#### Arguments

test\_measurement

Measured MIC to standardise
Measured QC MIC to standardise to
control strain identifier (usually ATCC)
antibiotic name (will be coerced to AMR::as.ab)
Where the target MIC is a range, prefer the upper value in the range
Ignore NA (returns AMR::NA_mic_)
Guideline to use (EUCAST or CLSI)
Guideline year (version)
Force into MIC-compatible format after standardisation

## Value

AMR::mic vector

## Examples

subset.mic\_validation Subset MIC validation object

#### Description

Subset MIC validation object

## Usage

```
## S3 method for class 'mic_validation'
subset(x, subset, ...)
```

## Arguments

х	mic_validation object
subset	logical expression to subset by
	additional arguments

#### Value

mic\_validation object

## Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
ab <- AMR::as.ab(c("AMK", "AMK", "CIP", "CIP"))
mo <- AMR::as.mo(c("E. coli", "E. coli", "P. mirabilis", "P. mirabilis"))
val <- compare_mic(gold_standard, test, ab, mo)
subset(val, ab == AMR::as.ab("AMX"))
subset(val, mo == AMR::as.mo("E. coli"))</pre>
```

summary.mic\_validation

Summary of MIC validation results

## Description

Summarise the results of an MIC validation generated using compare\_mic().

#### Usage

```
## S3 method for class 'mic_validation'
summary(object, ...)
```

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#### Arguments

object	S3 mic_validation object
	further optional parameters

## Value

S3 mic\_validation\_summary object

## Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
summary(val)
# or, for more detailed results
as.data.frame(summary(val))</pre>
```

table

Table

## Description

Table

## Usage

```
table(x, ...)
## Default S3 method:
table(x, ...)
## S3 method for class 'mic_validation'
table(
    x,
    format = "flextable",
    fill_dilutions = TRUE,
    bold = TRUE,
    ea_color = NULL,
    gold_standard_name = "Gold Standard",
    test_name = "Test",
    ...
)
```

## Arguments

х	mic_validation S3 object	
	further arguments	
format	simple or flextable	
fill_dilutions	Fill dilutions that are not present in the data in order to match the y- and x- axes	
bold	Bold cells where essential agreement is TRUE	
ea_color	Background color for essential agreement cells	
gold_standard_name		
	Name of the gold standard to display in output	
test_name	Name of the test to display in output	

#### Value

table or flextable object

## Examples

```
gold_standard <- c("<0.25", "8", "64", ">64")
test <- c("<0.25", "2", "16", "64")
val <- compare_mic(gold_standard, test)
table(val)</pre>
```

tidy\_patric\_meta\_data Tidy PATRIC data

## Description

Tidy PATRIC data

## Usage

```
tidy_patric_meta_data(
    x,
    prefer_more_resistant = TRUE,
    as_ab = TRUE,
    filter_abx = NULL
)
```

## Arguments

х	PATRIC database loaded using MIC::load_patric_db
prefer_more_r	resistant
	High MICs, narrow zones, or resistant phenotypes will be preferred where mul- tiple reported for the same isolate
as_ab	convert antibiotics to AMR::ab class (column names are antibiotic codes)
filter_abx	filter antibiotics of interest, provided as a vector of antibiotics character names/codes, or ideally, as AMR::ab classes, created using AMR::as.ab

## Value

Tidy data, with antimicrobials in wide format, column names describing methodology ("mic\_", "disk\_", "pheno\_"). S3 class "tidy\_patric\_db".

#### Examples

```
db <- data.frame(genome_id = 1,
            genome_name = "E. coli",
            antibiotic = "amoxicillin",
            measurement = 2.0,
            measurement_unit = "mg/L",
            laboratory_typing_method = "Agar dilution",
            resistant_phenotype = "R")
db <- load_patric_db(db)
tidy_patric_meta_data(db)
```

train\_test\_filesystem Organise files into a train-test filesystem

## Description

Organise files into a train-test filesystem

## Usage

```
train_test_filesystem(
   path_to_files,
   file_ext,
   split = 0.8,
   train_folder = "train",
   test_folder = "test",
   shuffle = TRUE,
   overwrite = FALSE
)
```

#### Arguments

path_to_files	directory containing files
file_ext	file extension to filter
split	training data split
train_folder	name of training folder (subdirectory), will be created if does not exist
test_folder	name of testing folder (subdirectory), will be created if does not exist
shuffle	randomise files when splitting (if FALSE, files will be sorted by filename prior to splitting)
overwrite	force overwrite of files that already exist

## Value

named vector of train and test directories

## Examples

```
set.seed(123)
# create 10 random DNA files
tmp_dir <- tempdir()</pre>
# remove any existing .fna files
file.remove(
  list.files(tmp_dir, pattern = "*.fna", full.names = TRUE)
)
for (i in 1:10) {
writeLines(paste0(">", i, "\n", paste0(sample(c("A", "T", "C", "G"),
 100, replace = TRUE), collapse = "")), file.path(tmp_dir, paste0(i, ".fna")))
}
# split files into train and test directories
paths <- train_test_filesystem(tmp_dir,</pre>
                                file_ext = "fna",
                                split = 0.8,
                                shuffle = TRUE,
                                overwrite = TRUE)
list.files(paths[["train"]])
list.files(paths[["test"]])
```

```
unsqueezed_index_to_str
```

Get str conversion of unsqueezed kmer using index

## Description

Get str conversion of unsqueezed kmer using index

#### Usage

```
unsqueezed_index_to_str(x, k, starting_index = 1L)
```

#### Arguments

х	integer vector of kmer indices
k	kmer length
<pre>starting_index</pre>	starting index (libsvm is usually indexed starting at 1)

#### Value

vector of unsqueezed kmer strings

#### Examples

unsqueezed\_index\_to\_str(2, k = 3)

unsqueezed\_mers Generates all permutations of unsqueezed kmers

#### Description

Generates all permutations of unsqueezed kmers

#### Usage

unsqueezed\_mers(k = 3L)

#### Arguments

k kmer length

#### Value

vector of unsqueezed kmers

#### Examples

unsqueezed\_mers(3)

xgb.cv.lowmem

Low memory cross-validation wrapper for XGBoost

#### Description

This function performs similar operations to xgboost::xgb.cv, but with the operations performed in a memory efficient manner. Unlike xgboost::xgb.cv, this version does not load all folds into memory from the start. Rather it loads each fold into memory sequentially, and trains trains each fold using xgboost::xgb.train. This allows larger datasets to be cross-validated.

The main disadvantage of this function is that it is not possible to perform early stopping based the results of all folds. The function does accept an early stopping argument, but this is applied to each fold separately. This means that different folds can (and should be expected to) train for a different number of rounds.

This function also allows for a train-test split (as opposed to multiple) folds. This is done by providing a value of less than 1 to nfold, or a list of 1 fold to folds. This is not possible with xg-boost::xgb.cv, but can be desirable if there is downstream processing that depends on an xgb.cv.synchromous object (which is the return object of both this function and xgboost::xgb.cv).

Otherwise, where possible this function tries to return the same data structure as xgboost::xgb.cv, with the exception of callbacks (not supported as a field within the return object). To save models, use the save\_models argument, rather than the cb.cv.predict(save\_models = TRUE) callback.

xgb.cv.lowmem

## Usage

```
xgb.cv.lowmem(
 params = list(),
  data,
  nrounds,
  nfold,
  label = NULL,
 missing = NA,
 prediction = FALSE,
 metrics = list(),
 obj = NULL,
 feval = NULL,
  stratified = TRUE,
  folds = NULL,
  train_folds = NULL,
 verbose = 1,
 print_every_n = 1L,
 early_stopping_rounds = NULL,
 maximize = NULL,
 save_models = FALSE,
  . . .
)
```

## Arguments

params	parameters for xgboost
data	DMatrix or matrix
nrounds	number of training rounds
nfold	number of folds, or if < 1 then the proportion will be used as the training split in a train-test split
label	data labels (alternatively provide with DMatrix)
missing	handling of missing data (see xgb.cv)
prediction	return predictions
metrics	evaluation metrics
obj	custom objective function
feval	custom evaluation function
stratified	whether to use stratified folds
folds	custom folds
train_folds	custom train folds
verbose	verbosity level
print_every_n	print every n iterations
early_stopping_	rounds
	early stopping rounds (applied to each fold)

maximize	whether to maximize the evaluation metric
save_models	whether to save the models
	additional arguments passed to xgb.train

## Value

xgb.cv.synchronous object

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