Package ‘SomaDataIO’

March 15, 2023

Type  Package
Title  Input/Output ‘SomaScan’ Data
Version  6.0.0
Description  Load and export ‘SomaScan’ data via the
’SomaLogic Operating Co., Inc.’ proprietary text file
called an ADAT (*.adat'). For file format see
The package also exports auxiliary functions for
manipulating, wrangling, and extracting relevant
information from an ADAT object once in memory.
License  MIT + file LICENSE
BugReports  https://github.com/SomaLogic/SomaDataIO/issues
Depends  R (>= 4.1.0)
Imports  cli, crayon, dplyr (>= 1.0.6), lifecycle (>= 1.0.0), magrittr
        (>= 2.0.1), methods, readxl (>= 1.3.1), tibble (>= 3.1.2),
tidyrr (>= 1.1.3), usethis (>= 2.0.1)
Suggests  Biobase, ggplot2, knitr, recipes, rmarkdown, spelling,
testthat (>= 3.0.0), withr
VignetteBuilder  knitr
Copyright  SomaLogic Operating Co., Inc. 2023
Encoding  UTF-8
Language  en-US
LazyData  true
LazyDataCompression  xz
LazyLoad  true
Config/testthat/edition  3
RoxygenNote  7.2.3
NeedsCompilation  no
adat2eSet

Convert ADAT to ExpressionSet Object

Description

Utility to convert a SomaLogic soma_adat object to an ExpressionSet object via the Biobase package from Bioconductor: https://www.bioconductor.org/packages/release/bioc/html/Biobase.html.

Usage

adat2eSet(adat)
Arguments

adat A soma_adat class object as read into the R environment using read_adat().

Details

The Biobase package is required and must be installed from Bioconductor via the following at the R console:

```r
if (!requireNamespace("BiocManager", quietly = TRUE)) {
  install.packages("BiocManager")
}
BiocManager::install("Biobase", version = remotes::bioc_version())
```

Value

A Bioconductor object of class ExpressionSet.

Author(s)

Stu Field

References

https://bioconductor.org/install/

See Also

Other eSet: pivotExpressionSet()

Examples

```r
eSet <- adat2eSet(example_data)
class(eSet)
eSet

ft <- Biobase::exprs(eSet)
head(ft[, 1:10L], 10L)
```

Description

In a standard SomaLogic ADAT, the section of information that sits directly above the measurement data (RFU data matrix) is the column meta data (Col.Meta), which contains detailed information and annotations about the analytes, SeqId(), and their targets. See section below for further information about available fields and their descriptions. Use getAnalyteInfo() to obtain an object containing this information for programmatic analyses, and use getMeta() to obtain the column names representing the row-specific meta data about the samples (see section below).
**Col Meta (Analyte Annotations)**

Information describing the *analytes* is found to the above the data matrix in a standard SomaLogic ADAT. This information may consist of the any or all of the following:

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>SeqId</td>
<td>SomaLogic sequence identifier</td>
<td>2182-54</td>
</tr>
<tr>
<td>SeqidVersion</td>
<td>Version of SOMAmer sequence</td>
<td>2</td>
</tr>
<tr>
<td>SomaId</td>
<td>Target identifier, of the form SLnnnnnn (8 characters in length)</td>
<td>SL0003</td>
</tr>
<tr>
<td>TargetFullname</td>
<td>Target name curated for consistency with UniProt name</td>
<td>Complete</td>
</tr>
<tr>
<td>Target</td>
<td>SomaLogic Target Name</td>
<td>C4b</td>
</tr>
<tr>
<td>UniProt</td>
<td>UniProt identifier(s)</td>
<td>P0C0L-</td>
</tr>
<tr>
<td>EntrezGeneID</td>
<td>Entrez Gene Identifier(s)</td>
<td>720 721</td>
</tr>
<tr>
<td>EntrezGeneSymbol</td>
<td>Entrez Gene Symbol names</td>
<td>C4A C4B</td>
</tr>
<tr>
<td>Organism</td>
<td>Protein Source Organism</td>
<td>Human</td>
</tr>
<tr>
<td>Units</td>
<td>Relative Fluorescence Units</td>
<td>RFU</td>
</tr>
<tr>
<td>Type</td>
<td>SOMAmer target type</td>
<td>Protein</td>
</tr>
<tr>
<td>Dilution</td>
<td>Dilution mix assignment</td>
<td>0.01%</td>
</tr>
<tr>
<td>PlateScale_Reference</td>
<td>PlateScale reference value</td>
<td>1378.85</td>
</tr>
<tr>
<td>CalReference</td>
<td>Calibration sample reference value</td>
<td>1378.85</td>
</tr>
<tr>
<td>medNormRef_ReferenceRFU</td>
<td>Median normalization reference value</td>
<td>490.342</td>
</tr>
<tr>
<td>Cal_V4_&lt;YY&gt;<em>&lt;SSS&gt;</em>&lt;PPP&gt;</td>
<td>Calibration scale factor (for given Year_Study_Plate)</td>
<td>0.64</td>
</tr>
<tr>
<td>CalCheck</td>
<td>QC acceptance criteria across all plates/sets</td>
<td>PASS</td>
</tr>
<tr>
<td>QcReference_&lt;LLLLL&gt;</td>
<td>QC sample reference value (for given QC lot)</td>
<td>PASS</td>
</tr>
<tr>
<td>CalQcRatio_V4_&lt;YY&gt;<em>&lt;SSS&gt;</em>&lt;PPP&gt;</td>
<td>Post calibration median QC ratio to reference (for given Year_Study_Plate)</td>
<td>1.04</td>
</tr>
</tbody>
</table>

**Row Meta (Sample Annotations)**

Information describing the *samples* is typically found to the left of the data matrix in a standard SomaLogic ADAT. This information may consist of clinical information provided by the client, or run-specific diagnostic information included for assay quality control. Below are some examples of what may be present in this section:

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>PlateId</td>
<td>Plate identifier</td>
<td>V4-18-004_001, V4-18-004_002</td>
</tr>
<tr>
<td>ScannerID</td>
<td>Scanner used to analyze slide</td>
<td>SG12064173, SG14374437</td>
</tr>
<tr>
<td>PlatePosition</td>
<td>Location on 96 well plate (A1-H12)</td>
<td>A1, H12</td>
</tr>
<tr>
<td>SlideId</td>
<td>Agilent slide barcode</td>
<td>2.58E+11</td>
</tr>
<tr>
<td>Subarray</td>
<td>Agilent subarray (1 – 8)</td>
<td>1.8</td>
</tr>
<tr>
<td>SampleId</td>
<td>1st form is Subject Identifier, 2nd form (calibrators, buffers)</td>
<td>2031</td>
</tr>
<tr>
<td>SampleType</td>
<td>1st form for clinical samples (Sample), 2nd form as above</td>
<td>Sample, QC, Calibrator, Buffer</td>
</tr>
<tr>
<td>PercentDilution</td>
<td>Highest concentration the SOMAmer dilution groups</td>
<td>20</td>
</tr>
<tr>
<td>SampleMatrix</td>
<td>Sample matrix</td>
<td>Plasma-PPT</td>
</tr>
<tr>
<td>Barcode</td>
<td>1D Barcode of aliquot</td>
<td>S622225</td>
</tr>
<tr>
<td>Barcode2d</td>
<td>2D Barcode of aliquot</td>
<td>1.91E+08</td>
</tr>
<tr>
<td>SampleNotes</td>
<td>Assay team sample observation</td>
<td>Cloudy, Low sample volume, Reddish</td>
</tr>
<tr>
<td>SampleDescription</td>
<td>Supplemental sample information</td>
<td>Plasma QC 1</td>
</tr>
<tr>
<td>AssayNotes</td>
<td>Assay team run observation</td>
<td>Beads aspirated, Leak/Hole, Smear</td>
</tr>
</tbody>
</table>
### diffAdats

**Diff Two ADAT Objects**

**Description**

Diff tool for the differences between two `soma_adat` objects. When diffs of the table values are interrogated, **only** the intersect of the column meta data or feature data is considered.

**Usage**

```r
diffAdats(adat1, adat2, tolerance = 1e-06)
```

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>adat1, adat2</td>
<td>Two <code>soma_adat</code> objects to compare.</td>
</tr>
<tr>
<td>tolerance</td>
<td>Numeric &gt; 0. Differences smaller than tolerance are not triggered. See <code>all.equal()</code></td>
</tr>
</tbody>
</table>
getAnalyteInfo

Value

NULL, invisibly. Called for side effects.

Note

Only diffs of the column name intersect are reported.

Author(s)

Stu Field

Examples

```r
# subset 'example_data' for speed
# all SeqIds from 2000 -> 2999
seqs <- grep("seq\[20-9]\{3\}"., names(example_data), value = TRUE)
ex_data_small <- head(example_data[, c(getMeta(example_data), seqs)], 10L)
dim(ex_data_small)

# no diff to itself
diffAdats(ex_data_small, ex_data_small)

# remove random column
rm <- withr::with_seed(123, sample(1:ncol(ex_data_small), 1))
diffAdats(ex_data_small, ex_data_small[, -rm])

# randomly shuffle Subarray
diffAdats(ex_data_small, dplyr::mutate(ex_data_small, Subarray = sample(Subarray)))

# modify 2 RFUs randomly
new <- ex_data_small
new[5L, c(rm, rm + 1L)] <- 999
diffAdats(ex_data_small, new)
```

getAnalyteInfo          Get Analyte Annotation Information

Description

Uses the Col.Meta attribute (analyte annotation data that appears above the protein measurements in the *.adat text file) of a soma_adat object, adds the AptName column key, conducts a few sanity checks, and generates a "lookup table" of analyte data that can be used for simple manipulation and indexing of analyte annotation information. Most importantly, the analyte column names of the soma_adat (e.g. seq.XXXX.XX) become the AptName column of the lookup table and represents the key index between the table and soma_adat from which it comes.
`getAnalyteInfo` is a function that retrieves analyte information.

**Usage**
```
getAnalyteInfo(adat)
getTargetNames(tbl)
getFeatureData(adat)
```

**Arguments**
- `adat` is a `soma_adat` object (with intact attributes), typically created using `read_adat()`.
- `tbl` is a tibble object containing analyte target annotation information. This is usually the result of a call to `getAnalyteInfo()`.

**Value**
A tibble object with columns corresponding to the column meta data entries in the `soma_adat`. One row per analyte.

**Functions**
- `getTargetNames()`: creates a lookup table (or dictionary) as a named list object of `AptNames` and `Target` names in key-value pairs. This is a convenient tool to quickly access a `Target` name given the `AptName` in which the key-value pairs map the `seq.XXX.XX` to its corresponding `TargetName` in `tbl`. This structure which provides a convenient auto-completion mechanism at the command line or for generating plot titles.
- `getFeatureData()`: renamed in `SomaDataIO v5.1.0`. Exported (with life-cycle warning) to maintain backward compatibility. Please adjust your code accordingly.

**Author(s)**
Stu Field

**See Also**
`getAnalytes()`, `is_intact_attr()`, `read_adat()`

**Examples**
```
# Get Aptamer table
anno_tbl <- getAnalyteInfo(example_data)
anno_tbl

# Use `dplyr::group_by()`
dplyr::tally(dplyr::group_by(anno_tbl, Dilution)) # print summary by dilution

# Columns containing "Target"
anno_tbl |> dplyr::select(dplyr::contains("Target"))

# Rows of "Target" starting with MMP
```
getAnalytes

Return the feature names (i.e. the column names for SOMAmer reagent analytes) from a soma_adat. S3 methods also exist for these classes:

```r
#> [1] getAnalytes.character getAnalytes.data.frame getAnalytes.default
#> [4] getAnalytes.list getAnalytes.matrix getAnalytes.recipe
#> [7] getAnalytes.soma_adat
#> see '?methods' for accessing help and source code
```

`getMeta()` returns the inverse, a character vector of string names of non-analyte feature columns/variables, which typically correspond to the clinical ("meta") data variables. S3 methods exist for these classes:

```r
#> [1] getMeta.character getMeta.data.frame getMeta.default getMeta.list
#> [5] getMeta.matrix getMeta.soma_adat
#> see '?methods' for accessing help and source code
```

### Usage

```r
getAnalytes(x, n = FALSE, rm.controls = FALSE)
getMeta(x, n = FALSE)
getFeatures(x, n = FALSE, rm.controls = FALSE)
```

### Arguments

- **x**
  - Typically a soma_adat class object created using `read_adat()`.
- **n**
  - Logical. Return an integer corresponding to the `length` of the features?
- **rm.controls**
  - Logical. Should all control and non-human analytes (e.g. HybControls, Non-Human, Non-Biotin, Spuriomer) be removed from the returned value?
getAnalytes

Value

getAnalytes(): a character vector of ADAT feature ("analyte") names.

getMeta(): a character vector of ADAT clinical ("meta") data names.

For both, if n = TRUE, an integer corresponding to the length of the character vector.

Functions

- getFeatures(): renamed in SomaDataIO v5.1.0. Exported (with life-cycle warning) to maintain backward compatibility. Please adjust your code accordingly.

Author(s)

Stu Field

See Also

is.apt()

Examples

# RFU feature variables
apts <- getAnalytes(example_data)
head(apts)
getAnalytes(example_data, n = TRUE)

# vector string
bb <- getAnalytes(names(example_data))
all.equal(apts, bb)

# create some control sequences
# ~~~~~~~~~ Spuriomer ~~~ HybControl ~~~
apts2 <- c("seq.2053.2", "seq.2171.12", head(apts))
apts2
no_crtl <- getAnalytes(apts2, rm.controls = TRUE)
no_crtl
setdiff(apts2, no_crtl)

# clinical variables
mvec <- getMeta(example_data)
head(mvec, 10)
getMeta(example_data, n = TRUE)

# test 'data.frame' and 'character' S3 methods are identical
identical(getMeta(example_data), getMeta(names(example_data))) # TRUE
groupGenerics

Description

S3 group generic methods to apply group specific prototype functions to the RFU data only of soma_adat objects. The clinical meta data are not transformed and remain unmodified in the returned object (Math() and Ops()) or are ignored for the Summary() group. See groupGeneric().

Usage

```r
## S3 method for class 'soma_adat'
Math(x, ...)

antilog(x, base = 10)

## S3 method for class 'soma_adat'
Ops(e1, e2 = NULL)

## S3 method for class 'soma_adat'
Summary(..., na.rm = FALSE)

## S3 method for class 'soma_adat'
e1 == e2
```

Arguments

- `x` The soma_adat class object to perform the transformation.
- `...` Additional arguments passed to the various group generics as appropriate.
- `base` A positive or complex number: the base with respect to which logarithms are computed.
- `e1, e2` Objects.
- `na.rm` Logical. Should missing values be removed?

Value

A soma_adat object with the same dimensions of the input object with the feature columns transformed by the specified generic.

Functions

- `antilog()`: performs the inverse or anti-log transform for a numeric vector of soma_adat object. **note**: default is base = 10, which differs from the `log()` default base e.
- `Ops(soma_adat)`: performs binary mathematical operations on class soma_adat. See `Ops()`.
- `Summary(soma_adat)`: performs summary calculations on class soma_adat. See `Summary()`.
- `==` : compares left- and right-hand sides of the operator unless the RHS is also a soma_adat, in which case `diffAdats()` is invoked.
Math
Group members:

```r
> [1] "abs"  "acos"  "acosh"  "asin"  "asinh"  "atan"
> [7] "atanh" "ceiling" "cos"  "cosh"  "cospi"  "cummax"
> [13] "cummin" "cumprod" "cumsum" "digamma" "exp"  "expm1"
> [19] "floor"  "gamma"  "lgamma"  "log"  "log10"  "log1p"
> [25] "log2"  "sign"  "sin"  "sinh"  "sinpi"  "sqrt"
> [31] "tan"  "tanh"  "tanpi"  "trigamma"  "trunc"
```

Commonly used generics of this group include:

- `log()`, `log10()`, `log2()`, `antilog()`, `abs()`, `sign()`, `floor()`, `sqrt()`, `exp()`

Ops
Group members:

```r
> [1] "+"  "-"  "*"  "^"  "%/%"  "/"  "=="  ">
> [13] ">="
```

Note that for the `==` method if the RHS is also a `soma_adat`, `diffAdats()` is invoked which compares LHS vs. RHS. Commonly used generics of this group include:

- `+`, `-`, `*`, `/`, `^`, `==`, `>`, `<`

Summary
Group members:

```r
> [1] "all"  "any"  "max"  "min"  "prod"  "range"  "sum"
```

Commonly used generics of this group include:

- `max()`, `min()`, `range()`, `sum()`, `any()`

Author(s)
Stu Field

See Also
`groupGeneric()`, `getGroupMembers()`, `getGroup()`
Examples

# subset `example_data` for speed  
# all SeqIds from 2000 -> 2999
seqs <- grep("\^seq\.[0-9]{3}\$", names(example_data), value = TRUE)
ex_data_small <- head(example_data[, c(getMeta(example_data), seqs)], 10L)
dim(ex_data_small)
ex_data_small$seq.2991.9

# Math Generics:  
# --------------
# log-transformation
a <- log(ex_data_small)
a$seq.2991.9

b <- log10(ex_data_small)
b$seq.2991.9
isTRUE(all.equal(b, log(ex_data_small, base = 10)))

# floor
c <- floor(ex_data_small)
c$seq.2991.9

# square-root
d <- sqrt(ex_data_small)
d$seq.2991.9

# rounding
e <- round(ex_data_small)
e$seq.2991.9

# inverse log
antilog(1:4)
alog <- antilog(b)
all.equal(ex_data_small, alog)  # return `b` -> linear space

# Ops Generics:  
# ---------------
plus1 <- ex_data_small + 1
times2 <- ex_data_small * 2

sq <- ex_data_small^2
all.equal(sqrt(sq), ex_data_small)

gt100k <- ex_data_small > 100000
gt100k
ex_data_small == ex_data_small  # invokes diffAdats()
Description

This function runs a series of checks to determine if a "soma_adat" object has a complete set of attributes. If not, this indicates that the object has been modified since the initial `read_adat()` call. Checks for the presence of both "Header.Meta" and "Col.Meta" in the attribute names. These entries are added during the `read_adat()` call. Specifically, within these sections it also checks for the presence of the following entries:

"Header.Meta" section: "HEADER", "COL_DATA", and "ROW_DATA"
"Col.Meta" section: "SeqId", "Target", "Units", and "Dilution"

If any of the above they are altered or missing, FALSE is returned.

Usage

```r
is_intact_attr(adat, verbose = interactive())
is.intact.attributes(adat, verbose = interactive())
```

Arguments

- `adat` A `soma_adat` object to query.
- `verbose` Logical. Should the function call be run in `verbose` mode, printing relevant diagnostic call information to the console.

Value

Logical. TRUE if all checks pass, otherwise FALSE.
Functions

- `is.intact.attributes()`: has been superseded by a more convenient, current, tidy syntax.

See Also

`attributes()`

Examples

```r
# checking attributes
my_adat <- example_data
is_intact_attr(my_adat) # TRUE
is_intact_attr(my_adat[, -303L]) # doesn't break attrs; TRUE
attributes(my_adat)$Col.Meta$Target <- NULL # break attributes
is_intact_attr(my_adat, verbose = TRUE) # FALSE (Target missing)
```

---

**is_seqFormat**

**Test AptName Format**

Description

Test whether an object is in the new seq.XXXX.XX format.

Usage

```r
is_seqFormat(x)
```

Arguments

- `x` The object to be tested.

Value

A logical indicating whether `x` contains AptNames consistent with the new format, beginning with a seq. prefix.

Author(s)

Stu Field, Eduardo Tabacman

Examples

```r
# character S3 method
is_seqFormat(names(example_data)) # no; meta data not ^seq.
is_seqFormat(tail(names(example_data), -20L)) # yes

# soma_adat S3 method
is_seqFormat(example_data)
```
Description

The SomaScan platform continually improves its technical processes between assay versions; from changing reagents, liquid handling equipment, and increased analyte content. However, these upgrades can result in minute differences in RFU space for a given analyte, requiring a calibration (aka "lifting" or "bridging") to bring RFUs into a comparable space. This is accomplished by applying an analyte-specific scalar to each analyte RFU (ADAT column). The scalar values themselves are typically provided via *.xlsx file, which can be parsed via `read_annotations()`. See Details.

Usage

`lift_adat(adat, anno.tbl)`

Arguments

- `adat` A `soma_adat` class object.
- `anno.tbl` A table of annotations, typically the result of a call to `read_annotations()`.

Details

Lifting between various versions requires a specific annotations file containing scalars specific to desired lifting direction. For example, to "lift" between v4.1 -> v4.0, you must be working with SomaScan data in v4.1 space and an annotations file containing scalars to convert to v4.0. Likewise, "lifting" from v4.0 -> v4.1 requires a separate annotations file and a `soma_adat` from SomaScan v4.0.

Value

A "lifted" `soma_adat` object corresponding to the scaling reference in the `anno.tbl`. RFU values are rounded to 1 decimal to match standard SomaScan delivery format.

Examples

```r
# 'example_data' is SomaScan V4
adat <- head(example_data, 3L)
# read in version specific annotations file
# containing scaling values between assay versions
## Not run:
tbl <- read_annotations("path/to/annotations_file.xlsx")
## End(Not run)
# mock annotations table in lieu of '*.xlsx' file
tbl <- tibble::tibble(SeqId = getSeqId(getAnalytes(adat)),
```

```
"Plasma Scalar v4.0 to v4.1" = 1)  # scale by 1.0
# usually performed inside 'read_annotations()'
# assign valid testing version to annotations table
attr(tbl, "version") <- "SL-99999999-rev99-1999-01"

# perform the 'lifting'
lifted <- lift_adat(adat, tbl)

# 'tbl' contained all scalars = 1.0 (same RFUs)
all.equal(adat, lifted, check.attributes = FALSE)

# attributes updated to reflect the 'lift'
attr(lifted, "Header")$HEADER$ProcessSteps
attr(lifted, "Header")$HEADER$SignalSpace

loadAdatsAsList Load ADAT files as a list

Description
Load a series of ADATs and return a list of soma_adat objects, one for each ADAT file. collapseAdats() concatenates a list of ADATs from loadAdatsAsList(), while maintaining the relevant attribute entries (mainly the HEADER element). This makes writing out the final object possible without the loss of HEADER information.

Usage
loadAdatsAsList(files, collapse = FALSE, verbose = interactive(), ...)
collapseAdats(x)

Arguments
files A character string of files to load.
collapse Logical. Should the resulting list of ADATs be collapsed into a single ADAT object?
verbose Logical. Should the function call be run in verbose mode.
... Additional arguments passed to read_adat().
x A list of soma_adat class objects returned from loadAdatsAsList().

Details
Note 1: The default behavior is to "vertically bind" (rbind()) on the intersect of the column variables, with unique columns silently dropped.

Note 2: If "vertically binding" on the column union is desired, use bind_rows(), however this results in NAs in non-intersecting columns. For many files with little variable intersection, a sparse RFU-matrix will result (and will likely break ADAT attributes):
adats <- loadAdatsAsList(files)
union_adat <- dplyr::bind_rows(adats, .id = "SourceFile")
Value

A list of ADATs named by `files`, each a `soma_adat` object corresponding to an individual file in `files`. For `collapseAdats()`, a single, collapsed `soma_adat` object.

Author(s)

Stu Field

See Also

`read_adat()`

Other IO: `parseHeader()`, `read_adat()`, `soma_adat`, `write_adat()`

Examples

```r
# only 1 file in directory
dir(system.file("extdata", package = "SomaDataIO"))
files <- system.file("extdata", package = "SomaDataIO") |> rev()
adats <- loadAdatsAsList(files)
class(adats)

# collapse into 1 ADAT
collapsed <- collapseAdats(adats)
class(collapsed)

# Alternatively use `collapse = TRUE`
loadAdatsAsList(files, collapse = TRUE)
```

---

**parseHeader**

**SomaLogic ADAT parser**

Description

Parses the header section of an ADAT file.

Usage

`parseHeader(file)`

Arguments

- `file` Character. The elaborated path and file name of the *.adat file to be loaded into an R workspace environment.
pivotExpressionSet

Value

A list of relevant file information required by `read_adat()` in order to complete loading the ADAT file, including:

- **Header.Meta**: list of notes and other information about the adat
- **Col.Meta**: list of vectors that contain the column meta data about individual analytes, includes information about the target name and calibration and QC ratios
- **file_specs**: list of values of the file parsing specifications
- **row_meta**: character vector of the clinical variables; assay information that is included in the adat output along with the RFU data

Author(s)

Stu Field

See Also

Other IO: `loadAdatsAsList()`, `read_adat()`, `soma_adat`, `write_adat()`

Examples

```r
f <- system.file("extdata", "example_data10.adat", package = "SomaDataIO", mustWork = TRUE)
header <- parseHeader(f)
header
```

pivotExpressionSet  
*Convert to Long Format*

Description

Utility to convert an ExpressionSet class object from the "wide" data format to the "long" format via `pivot_longer()`. The `Biobase` package is required for this function.

Usage

`pivotExpressionSet(eSet)`

Arguments

- **eSet**: An ExpressionSet class object, created using `adat2eSet()`.

Value

A tibble consisting of the long format conversion of an ExpressionSet object.
**read_adat**

**Author(s)**
Stu Field

**See Also**
Other eSet: `adat2eSet()`

**Examples**

```r
# subset into a reduced mini-ADAT object
# 10 samples (rows)
# 5 clinical variables and 3 features (cols)
sub_adat <- example_data[1:10, c(1:5, 35:37)]
ex_set  <- adat2eSet(sub_adat)

# convert ExpressionSet object to long format
adat_long <- pivotExpressionSet(ex_set)
```

---

### Description

The `read_adat()` function reads a `.adat` file as a `data.frame`-like object into an R workspace environment. The class of the returned object is a `soma_adat` object.

**read.adat()** is a convenient backward compatibility alias for `read_adat()` to enable use of older versions of SomaDataIO. It will likely never go away completely, but you strongly encouraged to shift your code to use `read_adat()`.

**is.soma_adat()** checks whether an object is of class `soma_adat`. See **inherits()**.

### Usage

```r
read_adat(file, debug = FALSE, verbose = getOption("verbose"), ...)  
read.adat(file, debug = FALSE, verbose = getOption("verbose"), ...)  
is.soma_adat(x)
```

### Arguments

- **file**: Character. The elaborated path and file name of the `.adat` file to be loaded into an R workspace.
- **debug**: Logical. Used for debugging and development of an ADAT that fails to load, particularly out-of-spec, poorly modified, or legacy ADATs.
- **verbose**: Logical. Should the function call be run in verbose mode, printing relevant diagnostic call information to the console.
... Additional arguments passed ultimately to `read.delim()`, or additional arguments passed to either other S3 print or summary methods as required by those generics.

x An R object to test.

Value

A `data.frame`-like object of class `soma_adat` consisting of SomaLogic RFU (feature) data and clinical meta data as columns, and samples as rows. Row names are labeled with the unique ID "SlideId_Subarray" concatenation. The sections of the ADAT header (e.g., "Header.Meta", "Col.Meta", ...) are stored as attributes (e.g. `attributes(x)$Header.Meta`).

Logical. Whether `x` inherits from class `soma_adat`.

Author(s)

Stu Field

See Also

`read.delim()`

Other IO: `loadAdatsAsList()`, `parseHeader()`, `soma_adat`, `write_adat()`

Examples

```r
f <- system.file("extdata", "example_data10.adat",
    package = "SomaDataIO", mustWork = TRUE)
my_adat <- read_adat(f)

is.soma_adat(my_adat)
```

---

**read_annotations**

Import a SomaLogic Annotations File

Description

Import a SomaLogic Annotations File

Usage

`read_annotations(file)`

Arguments

file A path to an annotations file location. This is a sanctioned, versioned file provided by SomaLogic Operating Co., Inc. and should be an unmodified *.xlsx file.
Value
A tibble containing analyte-specific annotations and related information (e.g. lift/scale information), keyed on SomaLogic "SeqId" which is a unique analyte identifier.

Examples
```r
## Not run:
anno <- read_annotations("~/Desktop/SomaScan_V4.1_7K_Annotated_Content_20210616.xlsx")
## End(Not run)
```

---

Helpers for Working With Row Names

Description
Easily move row names to a column and vice-versa without the unwanted side-effects to object class and attributes. Drop-in replacement for `tibble::rownames_to_column()` and `tibble::column_to_rownames()` which can have undesired side-effects to complex object attributes. Does not import any external packages, modify the environment, or change the object (other than the desired column). When using `col2rn()`, if explicit row names exist, they are overwritten with a warning. `add_rowid()` does not affect row names, which differs from `tibble::rowid_to_column()`.

Usage
```r
rn2col(data, name = ".rn")
col2rn(data, name = ".rn")
has rn(data)
rm rn(data)
set rn(data, value)
add rowid(data, name = ".rowid")
```

Arguments
- `data` An object that inherits from class `data.frame`. Typically a `soma_adat` class object.
- `name` Character. The name of the column to move.
- `value` Character. The new set of names for the data frame. If duplicates exist they are modified on-the-fly via `make.unique()`.
Value

All functions attempt to return an object of the same class as the input with fully intact and unmodified attributes (aside from those required by the desired action). `has_rn()` returns a scalar logical.

Functions

- `rn2col()`: moves the row names of data to an explicit column whether they are explicit or implicit.
- `col2rn()`: is the inverse of `rn2col()`. If row names exist, they will be overwritten (with warning).
- `has_rn()`: returns a boolean indicating whether the data frame has explicit row names assigned.
- `rm_rn()`: removes existing row names, leaving only "implicit" row names.
- `set_rn()`: sets (and overwrites) existing row names for data frames only.
- `add_rowid()`: adds a sequential integer row identifier; starting at 1:nrow(data). It does not remove existing row names currently, but may in the future (please code accordingly).

Examples

```r
df <- data.frame(a = 1:5, b = rnorm(5), row.names = LETTERS[1:5])
df
rn2col(df)  # default name is `.rn`
rn2col(df, "AptName")  # pass `name =`

# moving columns
df$mtcars <- sample(names(mtcars), 5)
col2rn(df, "mtcars")  # with a warning

# Move back and forth easily
# Leaves original object un-modified
identical(df, col2rn(rn2col(df)))

# add "id" column
add_rowid(mtcars)

# remove row names
has_rn(mtcars)
mtcars2 <- rm_rn(mtcars)
has_rn(mtcars2)
```

SeqId

Working with SomaLogic SeqIds

Description

The SeqId is the cornerstone used to uniquely identify SomaLogic analytes. SeqIds follow the format `<Pool>-<Clone>_<Version>`, for example "1234-56_7" can be represented as:
See Details below for the definition of each sub-unit. The <Pool><Clone> combination is sufficient to uniquely identify a specific analyte and therefore versions are no longer provided (though they may be present in legacy ADATs). The tools below enable users to extract, test, identify, compare, and manipulate SeqIds across assay runs and/or versions.

Usage

getSeqId(x, trim.version = FALSE)

regexSeqId()

locateSeqId(x, trailing = TRUE)

seqId2Apt(x)

apt2seqId(x)

is.aapt(x)

is.SeqId(x)

matchSeqIds(x, y, order.by.x = TRUE)

getSeqIdMatches(x, y, show = FALSE)

Arguments

x Character. A vector of strings, usually analyte/feature column names, AptNames, or SeqIds. For seqId2Apt(), a vector of SeqIds. For apt2seqId(), a character vector containing SeqIds. For matchSeqIds(), a vector of pattern matches containing SeqIds. Can be AptNames with GeneIDs, the seq.XXXX format, or even "naked" SeqIds.

trim.version Logical. Whether to remove the version number, i.e. "1234-56_7" -> "1234-56". Primarily for legacy ADATs.

trailing Logical. Should the regular expression explicitly specify trailing SeqId pattern match, i.e. "regex$"? This is the most common case and the default.

y Character. A second vector of AptNames containing SeqIds to match against those in contained in x. For matchSeqIds() these values are returned if there are matching elements.

order.by.x Logical. Order the returned character string by the x (first) argument?

show Logical. Return the data frame visibly?

Details
Pool: ties back to the original well during SELEX
Clone: ties to the specific sequence within a pool
Version: refers to custom modifications (optional/defunct)

AptName a SeqId combined with a string, usually a GeneId- or seq.-prefix, for convenient, human-readable manipulation from within R.

Value

`getSeqId()`: a character vector of SeqIds captured from a string.

`regexSeqId()`: a regular expression (regex) string pre-defined to match SomaLogic the SeqId pattern.

`locateSeqId()`: a data frame containing the start and stop integer positions for SeqId matches at each value of x.

`seqid2apt()`: a character vector with the seq.* prefix, i.e. the inverse of `getSeqId()`.

`apt2seqid()`: a character vector of SeqIds. `is.SeqId()` will return TRUE for all elements.

`is.apt()`, `is.SeqId()`: Logical. TRUE or FALSE.

`matchSeqIds()`: a character string corresponding to values in y of the intersect of x and y. If no matches are found, character(0).

`getSeqIdMatches()`: a n x 2 data frame, where n is the length of the intersect of the matching SeqIds. The data frame is named by the passed arguments, x and y.

Functions

- `getSeqId()`: extracts/captures the the SeqId match from an analyte column identifier, i.e. column name of an ADAT loaded with `read_adat()`. Assumes the SeqId pattern occurs at the end of the string, which for the vast majority of cases will be true. For edge cases, see the trailing argument to `locateSeqId()`.
- `regexSeqId()`: generates a pre-formatted regular expression for matching of SeqIds. Note the trailing match, which is most commonly required, but `locateSeqId()` offers an alternative to match anywhere in a string. Used internally in many utility functions
- `locateSeqId()`: generates a data frame of the positional SeqId matches. Specifically designed to facilitate SeqId extraction via `substr()`. Similar to `stringr::str_locate()`.
- `seqid2apt()`: converts a SeqId into anonymous-AptName format, i.e. 1234-56 -> seq.1234.56. Version numbers (1234-56_ver) are always trimmed when present.
- `apt2seqid()`: converts an anonymous-AptName into SeqId format, i.e. seq.1234.56 -> 1234-56. Version numbers (seq.1234.56.ver) are always trimmed when present.
- `is.apt()`: regular expression match to determine if a string contains a SeqId, and thus is probably an AptName format string. Both legacy EntrezGeneSymbol-SeqId combinations or newer so-called "anonymous-AptNames" formats (seq.1234.45) are matched.
- `is.SeqId()`: tests for SeqId format, i.e. values returned from `getSeqId()` will always return TRUE.
- `matchSeqIds()`: matches two character vectors on the basis of their intersecting SeqIds. Note that elements in y not containing a SeqId regular expression are silently dropped.
**getSeqIdMatches()**: matches two character vectors on the basis of their intersecting SeqIds only (irrespective of the GeneID-prefix). This produces a two-column data frame which then can be used as to map between the two sets.

The final order of the matches/rows is by the input corresponding to the first argument (x).

By default the data frame is invisibly returned to avoid dumping excess output to the console (see the show = argument.)

**Author(s)**

Stu Field

**See Also**

`intersect()`

**Examples**

```r
tibble::tibble(orig = x, SeqId = getSeqId(x), SeqId_trim = getSeqId(x, TRUE), AptName = seqid2apt(SeqId))
```

- Logical Matching
  ```r
  is.apt("AGR2.4959.2") # TRUE
  is.apt("seq.4959.2") # TRUE
  is.apt("4959-2") # TRUE
  is.apt("AGR2") # FALSE
  ```

- SeqId Matching
  ```r
  x <- c("seq.4554.56", "seq.3714.49", "PlateId")
y <- c("Group", "3714-49", "Assay", "4554-56")
matchSeqIds(x, y)
matchSeqIds(x, y, order.by.x = FALSE)
```

- vector of features
  ```r
  feats <- getAnalytes(example_data)
  match_df <- getSeqIdMatches(feats[1:100], feats[90:500]) # 11 overlapping
  match_df
  ```

- SeqId & shuffle
  ```r
  a <- utils::head(feats, 15)
b <- withr::with_seed(99, sample(getSeqId(a))) # => SeqId & shuffle
  (getSeqIdMatches(a, b)) # sorted by first vector "a"`
SomaDataIO-deprecated  Deprecated function(s) of the SomaDataIO package

Description

These functions are provided for compatibility with older versions of the SomaDataIO package. They may eventually be completely removed, so please re-code your scripts accordingly.

Arguments

...  A simple argument pass-through to an alternative replacement function if available.

Details

meltExpressionSet() now use pivotExpressionSet()
getSomamers() now use getAnalytes()
getFeatures() now use getAnalytes()
getSomamerData() now use getAnalyteInfo()
getFeatureData() now use getAnalyteInfo()

Author(s)

Stu Field

Example Data and Objects

Description

The example_data object is intended to provide existing and prospective SomaLogic customers with example data to enable analysis preparation prior to receipt of SomaScan data, and also for those generally curious about the SomaScan data deliverable. It is not intended to be used as a control group for studies or provide any metrics for SomaScan data in general.

Format

elementary_data  a soma_adat parsed via read_adat() containing 192 samples (see below for breakdown of sample type). There are 5318 columns containing 5284 analyte features and 34 clinical meta data fields. These data have been pre-processed via the following steps:

• hybridization normalized (all samples)
• calibrators and buffers median normalized
SomaScanObjects

- plate scaled
- calibrated
- Adaptive Normalization by Maximum Likelihood (ANML) of QC and clinical samples

Note1: The Age and Sex (M/F) fields contain simulated values designed to contain biological signal.

**Note2:** The `SampleType` column contains sample source/type information and usually the `SampleType == Sample` represents the "client" samples.

**Note3:** The original source file can be found at [url(https://github.com/SomaLogic/SomaLogic-Data)]

ex_analytes character string of the analyte features contained in the soma_adat object, derived from a call to `getAnalytes()`.

ex_anno_tbl a lookup table corresponding to a transposed data frame of the "Col.Meta" attribute of an ADAT, with an index key field `AptName` included in column 1, derived from a call to `getAnalyteInfo()`.

ex_target_names A lookup table mapping `SeqId` feature names -> target names contained in example_data. This object (or one like it) is convenient at the console via auto-complete for labeling and/or creating plot titles on the fly.

Data Description

The example_data object contains a SomaScan V4 study from healthy normal individuals. The RFU measurements themselves and other identifiers have been altered to protect personally identifiable information (PII), but also retain underlying biological signal as much as possible. There are 192 total EDTA-plasma samples across two 96-well plate runs which are broken down by the following types:

- 170 clinical samples (client study samples)
- 10 calibrators (replicate controls for combining data across runs)
- 6 QC samples (replicate controls used to assess run quality)
- 6 Buffer samples (no protein controls)

Data Processing

The standard V4 data normalization procedure for EDTA-plasma samples was applied to this dataset. For more details on the data standardization process see the Data Standardization and File Specification Technical Note. General details are outlined above.

Source

[https://github.com/SomaLogic/SomaLogic-Data](https://github.com/SomaLogic/SomaLogic-Data)

SomaLogic Operating Co., Inc.
Examples

```r
# S3 print method
e.example_data

# print header info
print(example_data, show_header = TRUE)

class(example_data)

# Features/Analytes
head(ex_analytes, 20L)

# Feature info table (annotations)
ex_anno_tbl

# Search via `filter()`
dplyr::filter(ex_anno_tbl, grepl("MMP", Target))

# Lookup table -> targets
# MMP-9
ex_target_names$seq.2579.17

# gender hormone FSH
tapply(example_data$seq.3032.11, example_data$Sex, median)

# gender hormone LH
tapply(example_data$seq.2953.31, example_data$Sex, median)

# Target lookup
ex_target_names$seq.2953.31  # tab-completion at console

# Sample Type/Source
table(example_data$SampleType)

# Sex/Gender Variable
table(example_data$Sex)

# Age Variable
summary(example_data$Age)
```

---

**soma_adat**

The **soma_adat** Class and S3 Methods

#### Description

The **soma_adat** data structure is the primary internal R representation of SomaScan data. A **soma_adat** is automatically created via `read_adat()` when loading a *.adat* text file. It consists of a data.frame-like object with leading columns as clinical variables and SomaScan RFU data as the remaining variables. Two main attributes corresponding to analyte and SomaScan run information contained in the *.adat* file are added:
• Header.Meta: information about the SomaScan run, see `parseHeader()` or `attr(x, "Header.Meta")`
• Col.Meta: annotations information about the SomaScan reagents/analytes, see `getAnalyteInfo()` or `attr(x, "Col.Meta")`
• file_specs: parsing specifications for the ingested *.adat file
• row_meta: the names of the non-RFU fields. See `getMeta()`.

See `groupGenerics()` for a details on `Math()`, `Ops()`, and `Summary()` methods that dispatch on class `soma_adat`.

See `reexports()` for a details on re-exported S3 generics from other packages (mostly `dplyr` and `tidyr`) to enable S3 methods to be dispatched on class `soma_adat`.

Below is a list of all currently available S3 methods that dispatch on the `soma_adat` class:

```r
#> [1] [<- [[<- [[- ==
#> [6] $ $<- anti_join arrange count
#> [11] filter full_join getAnalytes getMeta group_by
#> [16] inner_join is_seqFormat left_join Math median
#> [21] merge mutate Ops print rename
#> [26] right_join sample_frac sample_n select semi_join
#> [31] separate slice_sample slice summary Summary
#> [36] transform ungroup unite
#> see '?methods' for accessing help and source code
```

The S3 `print()` method returns summary information parsed from the object attributes, if present, followed by a dispatch to the `tibble()` print method. Rownames are printed as the first column in the print method only.

The S3 `summary()` method returns the following for each column of the ADAT object containing SOMAmer data (clinical meta data is excluded):

• Target (if available)
• Minimum value
• 1st Quantile
• Median
• Mean
• 3rd Quantile
• Maximum value
• Standard deviation
• Median absolute deviation (`mad()`)
• Interquartile range (`IQR()`)

The S3 `Extract()` method is used for sub-setting a `soma_adat` object and relies heavily on the `[]` method that maintains the `soma_adat` attributes intact and subsets the `Col.Meta` so that it is consistent with the newly created object.

S3 extraction via `$` is fully supported, however, as opposed to the `data.frame` method, partial matching is not allowed for class `soma_adat`. 
S3 extraction via [[ is supported, however, we restrict the usage of [[ for soma_adat. Use only a numeric index (e.g. 1L) or a character identifying the column (e.g. "SampleID"). Do not use [[i,j]] syntax with [, use [ instead. As with $, partial matching is not allowed.

S3 assignment via [ is supported for class soma_adat.

S3 assignment via $ is fully supported for class soma_adat.

S3 assignment via [[] is supported for class soma_adat.

S3 median() is not currently supported for the soma_adat class, however a dispatch is in place to direct users to alternatives.

Usage

```r
## S3 method for class 'soma_adat'
print(x, show_header = FALSE, ...)

## S3 method for class 'soma_adat'
summary(object, tbl = NULL, digits = max(3L, getOption("digits") - 3L), ...)

## S3 method for class 'soma_adat'
x[i, j, drop = TRUE, ...]

## S3 method for class 'soma_adat'
x$name

## S3 method for class 'soma_adat'
x[[i, j, ..., exact = TRUE]]

## S3 replacement method for class 'soma_adat'
x[i, j, ...] <- value

## S3 replacement method for class 'soma_adat'
x$i, j, ... <- value

## S3 replacement method for class 'soma_adat'
x[[i, j, ...]] <- value

## S3 method for class 'soma_adat'
median(x, na.rm = FALSE, ...)
```

Arguments

- `x`, `object` A soma_adat class object.
- `show_header` Logical. Should all the Header Data information be displayed instead of the data frame (tibble) object?
- `...` Ignored.
- `tbl` An annotations table. If NULL (default), annotation information is extracted from the object itself (if possible). Alternatively, the result of a call to `getAnalyteInfo()`, from which Target names can be extracted.
digits  Integer. Used for number formatting with `signif()`.
i, j  Row and column indices respectively. If j is omitted, i is used as the column index.
drop  Coerce to a vector if fetching one column via `tbl[, j]`. Default FALSE, ignored when accessing a column via `tbl[j]`.
name  A name or a string.
extact  Ignored with a `warning()`.
value  A value to store in a row, column, range or cell.
na.rm  a logical value indicating whether NA values should be stripped before the computation proceeds.

Value

The set of S3 methods above return the `soma_adat` object with the corresponding S3 method applied.

See Also

`groupGenerics()`

Other IO: `loadAdatsAsList()`, `parseHeader()`, `read_adat()`, `write_adat()`

Examples

```r
# S3 print method
dmp <- example_data
# show the header info (no RFU data)
print(dmp, show_header = TRUE)

# S3 summary method
# MMP analytes (4)
mmps <- c("seq.2579.17", "seq.2788.55", "seq.2789.26", "seq.4925.54")
mmp_dmp <- dmp[, c("Sex", mmps)]
sweep(mmp_dmp)

# Summarize by group
mmp_dmp |>
  split(mmp_dmp$Sex) |>
  lapply(sweep)

# Alternatively pass annotations with Target info
anno <- getAnalyteInfo(mmp_dmp)
sweep(mmp_dmp, tbl = anno)
```

**transform**

*Scale Transform* soma_adat *Columns/Rows*

**Description**

Scale the *i*-th row or column of a soma_adat object by the *i*-th element of a vector. Designed to facilitate linear transformations of *only* the analyte/RFU entries by scaling the data matrix. If scaling the analytes/RFU (columns), *v* must have `getAnalytes(adat, n = TRUE)` elements. If scaling the samples (rows), *v* must have `nrow(_data)` elements.

**Usage**

```r
## S3 method for class 'soma_adat'
transform(_, data, v, dim = 2L, ...)
```

**Arguments**

- `_data` A soma_adat object.
- `v` A numeric vector of the appropriate length corresponding to `dim`.
- `dim` Integer. The dimension to apply elements of `v` to. 1 = rows; 2 = columns (default).
- `...` Currently not used but required by the S3 generic.

**Details**

Performs the following operations (quickly):

**Columns:**

\[ M_{n \times p} = A_{n \times p} * \text{diag}(v)_{p \times p} \]

**Rows:**

\[ M_{n \times p} = \text{diag}(v)_{n \times n} * A_{n \times p} \]

**Value**

A modified value of `_data` with either the rows or columns linearly transformed by `v`.

**Note**

This method is intentionally naive, and assumes the user has ordered `v` to match the columns/rows of `_data` appropriately. This must be done upstream.

**See Also**

`apply()`, `sweep()`
Examples

```r
# simplified example of underlying operations
M <- matrix(1:12, ncol = 4)
M

v <- 1:4
M %*% diag(v)  # transform columns

v <- 1:3
diag(v) %*% M  # transform rows

# dummy ADAT example:
v <- c(2, 0.5)  # double seq1; half seq2
adat <- data.frame(sample = paste0("sample_", 1:3),
  seq.1234.56 = c(1, 2, 3),
  seq.9999.88 = c(4, 5, 6) * 10)

adat

# 'soma_adat' to invoke S3 method dispatch
class(adat) <- c("soma_adat", "data.frame")
trans <- transform(adat, v)
data.frame(trans)
```

**write_adat**  
Write an ADAT to File

**Description**

One can write an existing modified internal ADAT (soma_adat R object) to an external file. However the ADAT object itself must have intact attributes, see `is_intact_attr()`.

**Usage**

```r
write_adat(x, file)
```

**Arguments**

- `x`  
  An object of class soma_adat. Both `is.soma_adat()` and `is_intact_attr()` must be TRUE.

- `file`  
  Character. File path where the object should be written. For example, extensions should be `.adat`.

**Details**

The ADAT specification no longer requires Windows end of line (EOL) characters ("\r\n"). The current EOL spec is "\n" which is commonly used in POSIX systems, like MacOS and Linux. Since the EOL affects the resulting checksum, ADATs written on other systems generate slightly
differing files. Standardizing to "\n" attempts to solve this issue. For reference, see the EOL encoding for operating systems below:
### write_adat

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Platform</th>
<th>Character</th>
</tr>
</thead>
<tbody>
<tr>
<td>LF</td>
<td>Linux</td>
<td>&quot;\n&quot;</td>
</tr>
<tr>
<td>CR</td>
<td>MacOS</td>
<td>&quot;\r&quot;</td>
</tr>
<tr>
<td>CRLF</td>
<td>DOS/Windows</td>
<td>&quot;\r\n&quot;</td>
</tr>
</tbody>
</table>

**Value**

Invisibly returns the input `x`.

**Author(s)**

Stu Field

**See Also**

- `read_adat()`, `is_intact_attr()`
- Other IO: `loadAdatsAsList()`, `parseHeader()`, `read_adat()`, `soma_adat`

**Examples**

```r
# trim to 1 sample for speed
adat_out <- head(example_data, 1L)

# attributes must(!) be intact to write
is_intact_attr(adat_out)

write_adat(adat_out, file = tempfile(fileext = ".adat"))
```
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