Package: chents (via r-universe)

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Type Package

Title Chemical Entities as R Objects

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Description Utilities for dealing with chemical entities and associated data as R objects. If Python and RDKit (> 2015.03) are installed and configured for use with 'reticulate', some basic chemoinformatics functions like the calculation of molecular weight and plotting of chemical structures in R graphics are available.

Imports webchem, R6, yaml, rsvg, grImport, reticulate

Suggests knitr, testthat, covr, devEMF

License GPL

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LazyData yes

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Contents

`chent` *An R6 class for chemical entities with associated data*

Description

The class is initialised with an identifier. Chemical information is retrieved from the internet. Additionally, it can be generated using RDKit if RDKit and its python bindings are installed.

Format

An `R6Class` generator object

Public fields

`identifier (character(1))`
: The identifier that was used to initiate the object, with attribute 'source'

`inchikey (character(1))`
: InChI Key, with attribute 'source'

`smiles (character())`
: SMILES code(s), with attribute 'source'

`mw (numeric(1))`
: Molecular weight, with attribute 'source'

`pubchem (list())`
: List of information retrieved from PubChem

`rdkit` List of information obtained with RDKit

`mol` <rdkit.Chem.rdchem.Mol> object

`svg` SVG code

`Picture` Graph as a `picture` object obtained using grImport

`Pict_font_size` Font size as extracted from the intermediate PostScript file

`pdf_height` Height of the MediaBox in the pdf after cropping

`p0` Vapour pressure in Pa

`cwsat` Water solubility in mg/L

`PUF` Plant uptake factor

`chyaml` List of information obtained from a YAML file

`TPs` List of transformation products as chent objects Add a transformation product to the internal list

`transformations` Data frame of observed transformations Add a line in the internal dataframe holding observed transformations

`soil_degradation` Dataframe of modelling DT50 values Add a line in the internal dataframe holding modelling DT50 values

`soil_ff` Dataframe of formation fractions

`soil_sorption` Dataframe of soil sorption data Add soil sorption data

Methods

Public methods:

- `chent$new()`
- `chent$try_pubchem()`
- `chent$get_pubchem()`
- `chent$get_rdkit()`
- `chent$get_chyaml()`
- `chent$add_p0()`
- `chent$add_cwsat()`
- `chent$add_PUF()`
- `chent$add_TP()`
- `chent$add_transformation()`
- `chent$add_soil_degradation()`
- `chent$add_soil_ff()`
- `chent$add_soil_sorption()`
- `chent$pdf()`
- `chent$png()`
- `chent$emf()`
- `chent$clone()`

Method `new()`**:** Creates a new instance of this R6 class.

Usage:

```
chent$new(
  identifier,
  smiles = NULL,
  inchikey = NULL,
  pubchem = TRUE,
  pubchem_from = c("name", "smiles", "inchikey"),
  rdkit = TRUE,
  template = NULL,
  chyaml = TRUE
)
```

Arguments:

`identifier` Identifier to be stored in the object

`smiles` Optional user provided SMILES code

`inchikey` Optional user provided InChI Key

`pubchem` Should an attempt be made to retrieve chemical information from PubChem via the webchem package?

`pubchem_from` Possibility to select the argument that is used to query pubchem

`rdkit` Should an attempt be made to retrieve chemical information from a local rdkit installation via python and the reticulate package?

`template` An optional SMILES code to be used as template for RDKit

`chyaml` Should we look for a identifier.yaml file in the working directory? Try to get chemical information from PubChem

Method `try_pubchem()`**:**

Usage:

```
chent$try_pubchem(query, from = "name")
```

Arguments:

`query` Query string to be passed to get_cid

`from` Passed to get_cid Get chemical information from PubChem for a known PubChem CID

Method `get_pubchem()`**:**

Usage:

```
chent$get_pubchem(pubchem_cid)
```

Arguments:

`pubchem_cid` CID Get chemical information from RDKit if available

Method `get_rdkit()`**:**

Usage:

```
chent$get_rdkit(template = NULL)
```

Arguments:

`template` Optional template specified as a SMILES code Obtain information from a YAML file

Method `get_chyaml()`**:**

Usage:

```
chent$get_chyaml(
  repo = c("wd", "local", "web"),
  chyaml = paste0(URLencode(self$identifier), ".yaml")
)
```

Arguments:

`repo` Should the file be looked for in the current working directory, a local git repository under `~/git/chyaml`, or from the web (not implemented).

`chyaml` The filename to be looked for Add a vapour pressure

Method `add_p0()`**:**

Usage:

```
chent$add_p0(p0, T = NA, source = NA, page = NA, remark = "")
```

Arguments:

`p0` The vapour pressure in Pa

`T` Temperature

`source` An acronym specifying the source of the information

`page` The page from which the information was taken

`remark` A remark Add a water solubility

Method `add_cwsat()`**:**

Usage:

```
chent$add_cwsat(cwsat, T = NA, pH = NA, source = NA, page = NA, remark = "")
```

Arguments:

`cwsat` The water solubility in mg/L

`T` Temperature

`pH` The pH value

`source` An acronym specifying the source of the information

`page` The page from which the information was taken

`remark` A remark Add a plant uptake factor

Method `add_PUF()`**:**

Usage:

```
chent$add_PUF(
  PUF = 0,
  source = "focus_generic_gw_2014",
  page = 41,
  remark = "Conservative default value"
)
```

Arguments:

`PUF` The plant uptake factor, a number between 0 and 1

`source` An acronym specifying the source of the information

`page` The page from which the information was taken

`remark` A remark

Method `add_TP()`**:**

Usage:

```
chent$add_TP(x, smiles = NULL, pubchem = FALSE)
```

Arguments:

`x` A chent object, or an identifier to generate a chent object

`smiles` A SMILES code for defining a chent object

`pubchem` Should chemical information be obtained from PubChem?

Method `add_transformation()`**:**

Usage:

```
chent$add_transformation(
  study_type,
  TP_identifier,
  max_occurrence,
  remark = "",
  source = NA,
  pages = NA
)
```

Arguments:

`study_type` A characterisation of the study type

`TP_identifier` An identifier of one of the transformation products in `self$TPs`

`max_occurrence` The maximum observed occurrence of the transformation product, expressed as a fraction of the amount that would result from stochiometric transformation

`remark` A remark

`source` An acronym specifying the source of the information

`pages` The page from which the information was taken

Method `add_soil_degradation()`**:**

Usage:

```
chent$add_soil_degradation(
  soils,
  DT50_mod,
  DT50_mod_ref,
  type = NA,
  country = NA,
  pH_orig = NA,
  pH_medium = NA,
  pH_H2O = NA,
  perc_OC = NA,
  temperature = NA,
  moisture = NA,
  category = "lab",
  formulation = NA,
  model = NA,
  chi2 = NA,
  remark = "",
  source,
  page = NA
)
```

Arguments:

`soils` Names of the soils

`DT50_mod` The modelling DT50 in the sense of regulatory pesticide fate modelling

`DT50_mod_ref` The normalised modelling DT50 in the sense of regulatory pesticide fate modelling

`type` The soil type

`country` The country (mainly for field studies)

pH_orig The pH stated in the study

pH_medium The medium in which this pH was measured

pH_H2O The pH extrapolated to pure water

perc_OC The percentage of organic carbon in the soil

temperature The temperature during the study in degrees Celsius

moisture The moisture during the study

category Is it a laboratory ('lab') or field study ('field')

formulation Name of the formulation applied, if it was not the technical active ingredient

model The degradation model used for deriving DT50_mod

chi2 The relative error as defined in FOCUS kinetics

remark A remark

source An acronym specifying the source of the information

page The page from which the information was taken

Method `add_soil_ff()`**:**

Usage:

```
chent$add_soil_ff(target, soils, ff = 1, remark = "", source, page = NA)
```

Arguments:

target The identifier(s) of the transformation product

soils The soil name(s) in which the transformation was observed

ff The formation fraction(s)

Method `add_soil_sorption()`**:**

Usage:

```
chent$add_soil_sorption(
  soils,
  Kf,
  Kfoc,
  N,
  type = NA,
  pH_orig = NA,
  pH_medium = NA,
  pH_H2O = NA,
  perc_OC = NA,
  perc_clay = NA,
  CEC = NA,
  remark = "",
  source,
  page = NA
)
```

Arguments:

Kf The sorption constant in L/kg, either linear (then N is 1) or according to Freundlich

Kfoc The constant from above, normalised to soil organic carbon

N The Freundlich exponent

`perc_clay` The percentage of clay in the soil

`CEC` The cation exchange capacity Write a PDF image of the structure

Method `pdf()`**:**

Usage:

```
chent$pdf(
  file = paste0(self$identifier, ".pdf"),
  dir = "structures/pdf",
  template = NULL
)
```

Arguments:

`file` The file to write to

`dir` The directory to write the file to

`template` A template expressed as SMILES to use in RDKit Write a PNG image of the structure

Method `png()`**:**

Usage:

```
chent$png(
  file = paste0(self$identifier, ".png"),
  dir = "structures/png",
  antialias = "gray"
)
```

Arguments:

`antialias` Passed to png Write an EMF image of the structure using emf

Method `emf()`**:**

Usage:

```
chent$emf(file = paste0(self$identifier, ".emf"), dir = "structures/emf")
```

Arguments:

`file` The file to write to

Method `clone()`**:** The objects of this class are cloneable with this method.

Usage:

```
chent$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

Examples

```
oct <- chent$new("1-octanol", smiles = "CCCCCCCCO", pubchem = FALSE)
print(oct)
if (!is.null(oct$Picture)) {
  plot(oct)
}
```

```
caffeine <- chent$new("caffeine")
print(caffeine)
if (!is.null(caffeine$Picture)) {
  plot(caffeine)
}
```

`draw_svg.chent` *Draw SVG graph from a chent object using RDKit*

Description

Draw SVG graph from a chent object using RDKit

Usage

```
draw_svg.chent(
  x,
  width = 300,
  height = 150,
  filename = paste0(names(x$identifier), ".svg"),
  subdir = "svg"
)
```

Arguments

`x`	The chent object to be plotted
`width`	The desired width in pixels
`height`	The desired height in pixels
`filename`	The filename
`subdir`	The path to which the file should be written

`pai` *An R6 class for pesticidal active ingredients and associated data*

Description

The class is initialised with an identifier which is generally an ISO common name. Additional chemical information is retrieved from the internet if available.

Format

An `R6Class` generator object

Super class

chents::chent -> pai

Public fields

iso ISO common name of the active ingredient according to ISO 1750

bcpc Information retrieved from the BCPC compendium available online at <pesticidecompendium.bcpc.org>
Creates a new instance of this R6 class.

Methods

Public methods:

- pai$new()
- pai$clone()

Method new(): This class is derived from chent. It makes it easy to create a chent from the ISO common name of a pesticide active ingredient, and additionally stores the ISO name as well as the complete result of querying the BCPC compendium using bcpc_query.

Usage:

```
pai$new(
  iso,
  identifier = iso,
  smiles = NULL,
  inchikey = NULL,
  bcpc = TRUE,
  pubchem = TRUE,
  pubchem_from = "auto",
  rdkit = TRUE,
  template = NULL,
  chyaml = TRUE
)
```

Arguments:

iso The ISO common name to be used in the query of the BCPC compendium

identifier Alternative identifier used for querying pubchem

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
pai$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
# On Travis, we get a certificate validation error,
# likely because the system (xenial) is so old,
# therefore don't run this example on Travis
```

```
if (Sys.getenv("TRAVIS") == "") {

atr <- pai$new("atrazine")
print(atr)
if (!is.null(atr$Picture)) {
  plot(atr)
}

}
```

`plot.chent` *Plot method for chent objects*

Description

Plot method for chent objects

Usage

```
## S3 method for class 'chent'
plot(x, ...)
```

Arguments

`x`	The chent object to be plotted
`...`	Further arguments passed to `grid.picture`

Examples

```
caffeine <- chent$new("caffeine")
print(caffeine)
if (!is.null(caffeine$Picture)) {
  plot(caffeine)
}
```

`ppp` *R6 class for a plant protection product with at least one active ingredient*

Description

Contains basic information about the active ingredients in the product

Format

An `R6Class` generator object.

Public fields

`name` The name of the product

`ais` A list of active ingredients

`concentrations` The concentration of the ais

`concentration_units` Defaults to g/L

`density` The density of the product

`density_units` Defaults to g/L Creates a new instance of this R6 class.

`...` Identifiers of the active ingredients

`concentrations` Concentrations of the active ingredients

`concentration_units` Defaults to g/L

`density` The density

`density_units` Defaults to g/L Printing method

Active bindings

`...` Identifiers of the active ingredients

Methods

Public methods:

- `ppp$new()`
- `ppp$print()`
- `ppp$clone()`

Method `new()`:

Usage:

```
ppp$new(
  name,
  ...,
  concentrations,
  concentration_units = "g/L",
  density = 1000,
  density_units = "g/L"
)
```

Method `print()`:

Usage:

```
ppp$print()
```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
ppp$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

print.chent *Printing method for chent objects*

Description

Printing method for chent objects

Usage

```
## S3 method for class 'chent'
print(x, ...)
```

Arguments

x	The chent object to be printed
...	Further arguments for compatibility with the S3 method

print.pai *Printing method for pai objects (pesticidal active ingredients)*

Description

Printing method for pai objects (pesticidal active ingredients)

Usage

```
## S3 method for class 'pai'
print(x, ...)
```

Arguments

x	The chent object to be printed
...	Further arguments for compatibility with the S3 method

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