

Package: chents (via r-universe)

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Type Package

Title Chemical Entities as R Objects

Version 0.4.2

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Description When working with data on chemical substances, we often need a reliable link between the data and the chemical identity of the substances. The R package 'chents' provides a way to define an R object corresponding to a chemically defined substances, i.e. a chemical entity and to collect related information. If Python and 'RDKit' (> 2015.03) are installed and configured for use with 'reticulate', some basic cheminformatics 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 (>= 3.0.0), covr, devEMF

License GPL

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LazyData yes

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Contents

chent	2
draw_svg.chent	9
pai	10
plot.chent	11
ppp	12
print.chent	13
print.pai	13
print.ppp	14

Index	15
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chent	<i>An R6 class for chemical entities with associated data</i>
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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 [grImport::Picture](#) object obtained using the `grImport` package
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
transformations Data frame of observed transformations
soil_degradation Dataframe of modelling DT50 values
soil_ff Dataframe of formation fractions
soil_sorption Dataframe of 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()`

`chent$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 = FALSE  
)
```

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?

chent\$try_pubchem(): Try to get chemical information from PubChem

Usage:

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

Arguments:

query Query string to be passed to [get_cid](#)

from Passed to [get_cid](#)

chent\$get_pubchem(): Get chemical information from PubChem for a known PubChem CID

Usage:

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

Arguments:

pubchem_cid CID

chent\$get_rdkit(): Get chemical information from RDKit if available

Usage:

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

Arguments:

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

chent\$get_chyaml(): Obtain information from a YAML file

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

chent\$add_p0(): Add a vapour pressure

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

```
chent$add_cwsat(): Add a water solubility
```

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 pH value

source An acronym specifying the source of the information

page The page from which the information was taken

remark A remark

```
chent$add_PUF(): Add a plant uptake factor
```

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

```
chent$add_TP(): Add a transformation product to the internal list
```

Usage:

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

Arguments:

x A [chent](#) object, or an identifier to generate a [chent](#) object

smiles Optional user provided SMILES code

pubchem Should chemical information be obtained from PubChem?

```
chent$add_transformation(): Add a line in the internal dataframe holding observed transformations
```

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 stoichiometric transformation
`remark` A remark
`source` An acronym specifying the source of the information
`pages` The pages from which the information was taken

`chent$add_soil_degradation()`: Add a line in the internal dataframe holding modelling DT50 values

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

chent\$add_soil_ff(): Add one or more formation fractions for degradation in soil

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)
 remark A remark
 source An acronym specifying the source of the information
 page The page from which the information was taken

chent\$add_soil_sorption(): Add soil sorption data

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:

soils Names of the soils
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
type The soil type
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
perc_clay The percentage of clay in the soil
CEC The cation exchange capacity
remark A remark
source An acronym specifying the source of the information
page The page from which the information was taken

chent\$pdf(): Write a PDF image of the structure

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 An optional SMILES code to be used as template for RDKit

chent\$png(): Write a PNG image of the structure

Usage:

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

Arguments:

file The file to write to
dir The directory to write the file to
antialias Passed to [png](#)

chent\$emf(): Write an EMF image of the structure using [emf](#)

Usage:

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

Arguments:

file The file to write to
 dir The directory to write the file to

chent\$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

```
# Don't run examples per default, as PubChem may be unavailable
## Not run:
caffeine <- chent$new("caffeine")
print(caffeine)
if (!is.null(caffeine$Picture)) {
  plot(caffeine)
}
oct <- chent$new("1-octanol", smiles = "CCCCCCCC", pubchem = FALSE)
print(oct)

## End(Not run)
```

 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

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](#).

Format

An [R6::R6Class](#) generator object

Super class

[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>

Methods

Public methods:

- [pai\\$new\(\)](#)
- [pai\\$clone\(\)](#)

[pai\\$new\(\)](#): Create a new pai object

Usage:

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

Arguments:

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

identifier Alternative identifier used for querying pubchem

smiles Optional user provided SMILES code
 inchikey Optional user provided InChI Key
 bcpc Should the BCPC compendium be queried?
 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

pai\$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

```

# Don't run examples per default, as PubChem may be unavailable
## Not run:
atr <- pai$new("atrazine")
print(atr)
if (!is.null(atr$Picture)) {
  plot(atr)
}
# We can also define pairs that are not found on the BCPC site
decanol <- pai$new("1-Decanol")
print(decanol)

## End(Not run)

```

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 [grImport::grid.picture](#)

Examples

```
# Don't run examples per default, as PubChem may be unavailable
## Not run:
caffeine <- chent$new("caffeine")
print(caffeine)
if (!is.null(caffeine$Picture)) {
  plot(caffeine)
}

## End(Not run)
```

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 [R6::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

Methods**Public methods:**

- [ppp\\$new\(\)](#)
- [ppp\\$clone\(\)](#)

[ppp\\$new\(\)](#): Creates a new instance of this [R6](#) class.

Usage:

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

Arguments:

name The name of the product
 ... 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

ppp\$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	<i>Printing method for chent objects</i>
-------------	--

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	<i>Printing method for pai objects (pesticidal active ingredients)</i>
-----------	--

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

`print.ppp`*Printing method for ppp objects (plant protection products)*

Description

Printing method for ppp objects (plant protection products)

Usage

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

Arguments

<code>x</code>	The object to be printed
<code>...</code>	Further arguments for compatibility with the S3 method

Index

`bcpq_query`, [10](#)

`chent`, [2](#), [5](#), [10](#)

`draw_svg.chent`, [9](#)

`emf`, [8](#)

`get_cid`, [4](#)

`grImport::grid.picture`, [11](#)

`grImport::Picture`, [2](#)

`pai`, [10](#)

`plot.chent`, [11](#)

`png`, [8](#)

`ppp`, [12](#)

`print.chent`, [13](#)

`print.pai`, [13](#)

`print.ppp`, [14](#)

`R6`, [3](#), [12](#)

`R6::R6Class`, [10](#), [12](#)

`R6Class`, [2](#)