

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 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, covr, devEMF

License GPL

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LazyData yes

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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 [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:

$p\theta$ 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 stoichiometric 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$new("1-octanol", smiles = "CCCCCCCC", pubchem = FALSE)
print(oct)
if (!is.null(oct$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

<code>x</code>	The chent object to be plotted
<code>width</code>	The desired width in pixels
<code>height</code>	The desired height in pixels
<code>filename</code>	The filename
<code>subdir</code>	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	<i>Printing method for chent objects</i>
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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>
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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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