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webchem: An R Package to Retrieve Chemical Information from the Web

Eduard Szöcs
Universität Koblenz-Landau

Ralf B. Schäfer
Universität Koblenz-Landau

Abstract

A wide range of chemical information is freely available online, including identifiers, experimental and predicted chemical properties. However, these data are scattered over various data sources and not easily accessible to researchers. Manual searching and downloading of such data is time-consuming and error-prone. We developed the open-source R package **webchem** that allows users to automatically query chemical data from currently 11 web sources. These cover a broad spectrum of information. The data are automatically imported into an R object and can directly be used in subsequent analyses. **webchem** enables easy, structured and reproducible data retrieval and usage from publicly available web sources. In addition, it facilitates data cleaning, identification and reporting of substances. Consequently, it reduces the time researchers need to spend on chemical data compilation.

Keywords: ecotoxicology, chemistry, data cleaning, web scraping, ropensci.

1. Introduction

Before each statistical analysis, data cleaning is often required to ensure good data quality. Data cleaning is the process of detecting errors and inconsistencies in data sets (Chapman 2005). In practice, the data cleaning step is often more time consuming than the subsequent statistical analysis, particularly, when the analysis relies on multiple data sources that need to be joined.

When dealing with chemical data sets (e.g. environmental monitoring data, toxicological data), a first step is often to validate the names of chemicals or to link them to unique codes that simplify subsequent querying and appending of compound-related physico-chemical or toxicological information. Several web sources provide chemical names or link them to unique codes (see also section *Data sources* below). However, manual searching for each compound,

often through a graphical web interface, is tedious, error-prone and not reproducible (Peng 2009).

To simplify, robustify and automate this task, i.e. to search and retrieve chemical information from the web, we created the **webchem** package for the free and open source R language (R Core Team 2016; Wehrens 2011). R is one of the most widely used software environments for data cleaning, analysing and visualising data, and supports full reproducibility of each step (Marwick 2016).

In the following, we describe the basic functionality of the package and demonstrate with a few use cases how to clean and retrieve new data with **webchem**.

2. Implementation and design details

The **webchem** package is written entirely in R and available under a MIT license. The development repository is hosted on GitHub (2016) and a stable version is released on the official R repository (CRAN 2016). **webchem** is part of the rOpenSci project (Boettiger *et al.* 2015), which aims at fully reproducible data analysis.

webchem follows best practices for scientific software (Wilson *et al.* 2014; Poisot 2015), namely: (i) a public available repository with easy collaboration and an issue tracker (via GitHub), (ii) a non-restrictive license, version control (git), (iii) an elaborate test-suite covering more than 90% of the relevant lines of code (currently ~1500 lines, using **testthat** (Wickham 2011)), (iv) continuous integration (via Travis-CI (2016) and AppVeyor (2016); testing on Linux & Windows with current and development R versions), (v) in-source documentation (using **roxygen2** (Wickham *et al.* 2015)) and (vi) compliance with a style guide (Wickham 2015a).

webchem builds on top of the following R packages: **RCurl** (Lang and team 2016) and **httr** (Wickham 2016) for data transfer, **stringr** (Wickham 2015c) for string handling, **xml2** (Wickham 2015d) and **rvest** (Wickham 2015b) for parsing HTML and XML, **jsonlite** (Ooms 2014) for parsing JSON, **rcdk** (Guha 2007) for parsing SMILES. For parsing molfiles we use a lightweight implementation of (Grabner *et al.* 2012).

Some data sources provide application programming interfaces (API). Web APIs define functions that allow accessing services and data via http and return data in a specific way. **webchem** uses the API of a data source provider, where this is provided. For sources where an API is lacking, data is directly searched and extracted from the web pages, analogous to manual interaction with a website.

Only few design decisions have been made: Each function name has a prefix and suffix separated by an underscore (Chamberlain and Szöcs 2013). They follow the format of `source_function`, e.g. `cs_compinfo` uses ChemSpider as source (see next section) to retrieve compound information. Some functions require querying first a unique identifier from the data source and then use this identifier to query further information. The prefix `get` is used to denote these functions, e.g. `get_csid` to retrieve the identifier used in ChemSpider.

webchem is friendly to the resources of data providers. Between each request there is a time-out of 0.3 to 2 seconds depending on the data source. Therefore, processing of larger data sets can take some time, but still represents a major improvement compared to manual look up. We provide a link to the *Terms of Use* of data providers in the documentation of each function and we encourage the users to read these before using **webchem**. Moreover, all

functions return an URL of the source, which can be used for (micro-)attribution.

3. Data sources

The backbone of **webchem** are data sources providing their data and functionality to the public. Currently, data can be retrieved from 11 sources. These cover a broad spectrum of available data, like identifiers, experimental and predicted properties and legal information (Figure 1, a detailed overview of all sources is included as supplement):

NIH Chemical Identifier Resolver (CIR) (NIH 2016) A web service that converts from and to various chemical identifiers.

Chemical Translation Service (CTS) (Wohlgemuth *et al.* 2010) A web service that converts from and to various chemical identifiers.

ETOX (UBA 2016) Information System Ecotoxicology and Environmental Quality Targets by the German Federal Environmental Agency. Provides basic identifiers, synonyms, ecotoxicological data and quality targets for different countries.

PAN Pesticide Database (PAN 2016) Information on pesticides - provides basic identifiers, ecotoxicological data and chemical properties.

SRC Physprop (Howard and Meylan 2016) Contains physical properties for over 41,000 chemicals. Physical properties collected from a wide variety of sources including experimental and modeled values.

PubChem (Kim *et al.* 2016) PubChem is a public repository for information on chemical substances, providing identifiers, properties and synonyms. We use an interface to the PUG-REST web service (Kim *et al.* 2015).

Wikidata (Wikipedia 2016) Wikipedia contains information entries for over 15,000 chemicals (Ertl *et al.* 2015). Currently **webchem** can query only chemical identifiers only.

Compendium of Pesticide Common Names (Wood 2016) The compendium provides information on pesticide common names, identifiers and classification.

ChemID*plus* (Tomasulo 2002) is a large web-based database provided by the National Library of Medicine. It provides identifiers, synonyms, toxicological data and chemical properties.

ChemSpider (Pence and Williams 2010) is a free chemical structure database providing access to over 40 million structures. It provides identifiers, properties and can also be used to convert identifiers.

OPSIN (Lowe *et al.* 2011) The Open Parser for Systematic IUPAC nomenclature is a chemical name interpreter and provides InChI and SMILES identifiers.

Though the data sources exhibit some overlap in the provided information, each has been selected because it provides unique information and we encourage the interested reader to

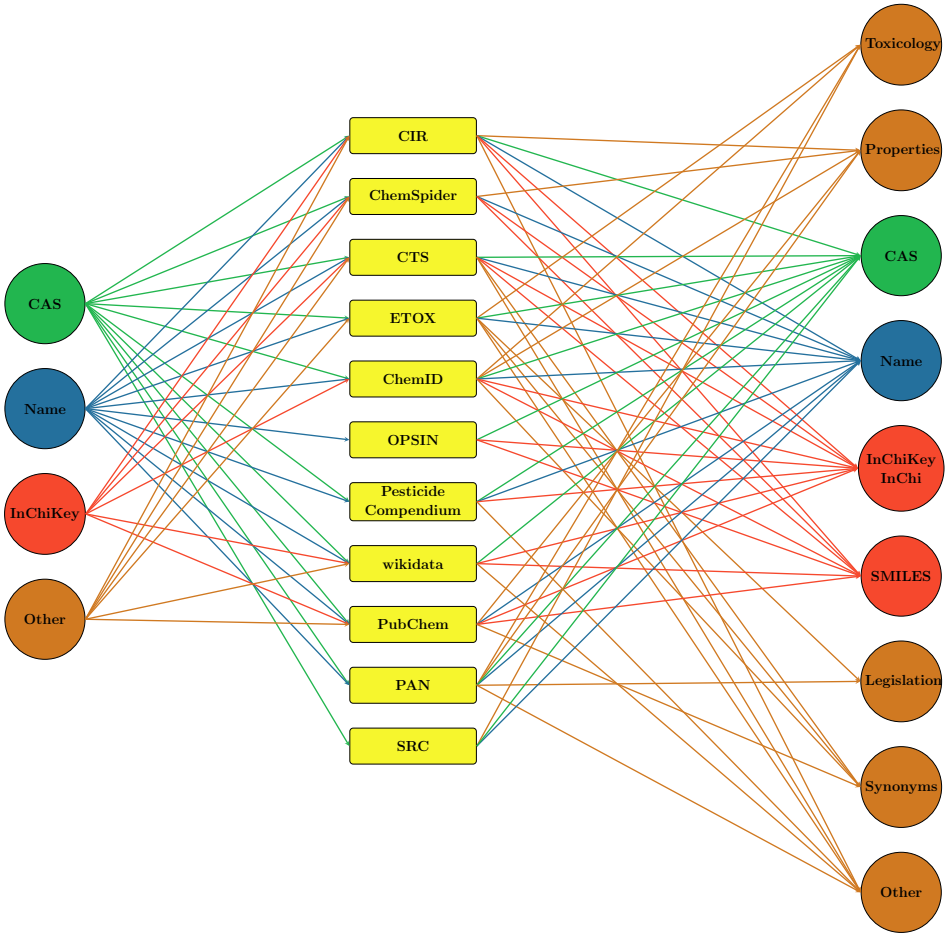

Figure 1: Overview of current data sources. Input and output possibilities currently implemented in the package.

consult the related source for details. However, we provide a brief overview in the Supporting Information.

4. Use cases

4.1. Installation

webchem can be easily installed and loaded from CRAN:

```
R> install.packages("webchem")
R> library("webchem")
```

The package is under active development. The latest development version is available from GitHub and also permanently available at Zenodo (2016). This document has been created using **webchem** version 0.1.

4.2. Sample data sets

To demonstrate the capabilities of **webchem** we use two small publicly available real world data sets. The data sets are only for demonstration purposes, have been slightly preprocessed (not shown) and are available through the package.

(i) `jagst`: This data set comprises environmental monitoring data of organic substances in the river Jagst, Germany, sampled in 2013. The data is publicly available and can be retrieved from LUBW (2016). It comprises concentrations (in μg / L) of 34 substances on 13 sampling occasions. First we load the data set and take a look at the first six rows:

```
R> data("jagst")
R> head(jagst)
```

```
        date          substance value qual
1 2013-01-04 2,4-Dimethylphenol 0.006    <
2 2013-01-29 2,4-Dimethylphenol 0.006    <
3 2013-02-26 2,4-Dimethylphenol 0.006    <
4 2013-03-26 2,4-Dimethylphenol 0.006    <
5 2013-04-23 2,4-Dimethylphenol 0.006    <
6 2013-05-22 2,4-Dimethylphenol 0.006    <
```

This data set identifies substances only by substance names. Values below the limit of quantification (LOQ) are indicated by a qualifier column.

(ii) `lc50`: This data consists of median acute lethal concentration for the water flea *Daphnia magna* in 48 h tests ($LC_{50,D.magna,48h}$) of 124 insecticides. The data has been retrieved from the EPA ECOTOX database (U.S. EPA 2016).

```
R> data("lc50")
R> head(lc50)
```

```
       cas        value
4  50-29-3    12.415277
12 52-68-6     1.282980
15 55-38-9    12.168138
18 56-23-5 35000.000000
21 56-38-2     1.539119
36 57-74-9    98.400000
```

This data set identifies the substances only by CAS numbers.

4.3. Query identifiers

The `jagst` data set covers 34 substances that are identified by (German) names. Merging and linking these to other tables is hampered by differences and ambiguity in compound names.

One possibility to resolve this, is to use different chemical identifiers allowing easy identification. There are several identifiers available, e.g. registry numbers like CAS or EC, database

identifiers like PubChemCID (Kim *et al.* 2016) or ChemSpiderID (Pence and Williams 2010), line notations like SMILES (Weininger 1990), InChI and InChiKey (Heller *et al.* 2015). In this first example we query several identifiers to create a table that can be used as (i) supplemental information to a research article or (ii) to facilitate subsequent matching with other data.

As we are are dealing with German substance names we start to query ETOX for CAS registry numbers. A common work flow when dealing with web resources is to 1) query a unique identifier of the source, 2) use this identifier to retrieve additional information and 3) extract the parts that are needed from the R object (Chamberlain and Szöcs 2013).

First we search for ETOX internal ID numbers using the substance names:

```
R> subs <- unique(jagst$substance)
R> ids <- get_etoxid(subs, match = 'best')
R> head(ids)
```

```
  etoxid                            match distance                  query
1   8668     2,4-Dimethylphenol ( 8668 )        0     2,4-Dimethylphenol
2   8494 4-Chlor-2-methylphenol ( 8494 )        0 4-Chlor-2-methylphenol
3   <NA>                             <NA>     <NA>     4-para-nonylphenol
4   8397                 Atrazin ( 8397 )        0                Atrazin
5   7240                  Benzol ( 7240 )        0                 Benzol
6   7331         Desethylatrazin ( 7331 )        0         Desethylatrazin
```

Only three substances could not be found in ETOX. Here we specify that only the *'best'* match (in terms of the Levenshtein distance between query and results) is returned. A manual check confirms appropriate matches. Other options include: *'all'* - returns all matches; *'first'* - returns only the first match (not necessarily the best match); *'ask'* - this enters an interactive mode, where the user is asked for a choice if multiple matches are found and *'na'* which returns `NA` in case of multiple matches.

We use these data to retrieve basic information on the substances.

```
R> etox_data <- etox_basic(ids$etoxid)
```

webchem always returns a named list (one entry for each substance) and the available information content can be very voluminous. Therefore, we provide extractor functions for the common identifiers: CAS, SMILES and InChIKeys.

```
R> etox_cas <- cas(etox_data)
R> head(etox_cas)
```

```
      8668        8494        <NA>        8397        7240        7331
"105-67-9" "1570-64-5"          NA "1912-24-9"   "71-43-2" "6190-65-4"
```

A variety of data are available and we cannot provide extractor functions for each of those. Therefore, if users need to extract other data, they have to write simple extractor functions (see following examples).

In the same manner we can now query other identifiers from other source using this CAS numbers (Figure 1), like PubChem

```
R> cids <- get_cid(etox_cas)
R> pc_data <- pc_prop(cids, properties = c('CanonicalSMILES'))
R> pc_smiles <- smiles(pc_data)
```

or ChemSpider

```
R> csids <- get_csid(etox_cas, token = token)
R> cs_data <- cs_compinfo(csids, token = token)
R> cs_inchikey <- inchikey(cs_data)
```

Finally, we combine the queried data into one data.frame

```
R> res <- data.frame(name = subs, cas = etox_cas, smiles = pc_smiles,
+    cid = pc_data$CID, inchikey = cs_inchikey, csid = cs_data$csid,
+    stringsAsFactors = FALSE)
```

Note, that in order to use the ChemSpider functions, a personal authentication key (`token`) is needed, which can be retrieved from the ChemSpider web page. We end up with a compound table containing many different identifiers (Table 1), allowing easy identification and merging with other data sets, e.g. the `lc50` data set based on CAS.

Name	CAS	SMILES	CID	InChIKey	CSID
2,4-Dimethylphenol	105-67-9	CC1=CC(...	7771	KUFFULV...	13839123
4-Chlor-2-methylphenol	1570-64-5	CC1=C(C...	14855	RHPUJHQ...	14165
4-para-nonylphenol	-	-	-	-	-
Atrazin	1912-24-9	CCNC1=N...	2256	MXWJVTO...	2169
Benzol	71-43-2	C1=CC=C...	241	UHOVQNZ...	236
Desethylatrazin	6190-65-4	CC(C)NC...	22563	DFWFIQK...	21157

Table 1: Identifiers for the jagst data sets as queried with **webchem**. Only the first 6 entries are shown. For SMILES and InChIKey only the first 7 characters are shown. - = not found.

4.4. Toxicity of different pesticide groups

Another question we might ask is *How does toxicity vary between insecticide groups?* Answering this question would require tedious look up of insecticide groups for each of the 124 CAS numbers in the `lc50` data set. The Compendium of Pesticide Common Names (Wood 2016) contains such information and can be easily queried using CAS numbers with **webchem**:

```
R> aw_data <- aw_query(lc50$cas, type = 'cas')
```

To extract the chemical group from the retrieved data set, we need to write a simple extractor function and apply this to the retrieved data:

```
R> igroup <- sapply(aw_data, function(y) y$subactivity[1])
R> igroup[1:3]
```

```
                                50-29-3
          "organochlorine insecticides"
                                52-68-6
            "phosphonate insecticides"
                                55-38-9
"phenyl organothiophosphate insecticides"
```

Figure 2 displays the result after some more data cleaning (see supplement for full code). Overall, it took only 5 R statements to retrieve, clean and plot the data using **ggplot2** (Wickham 2009).

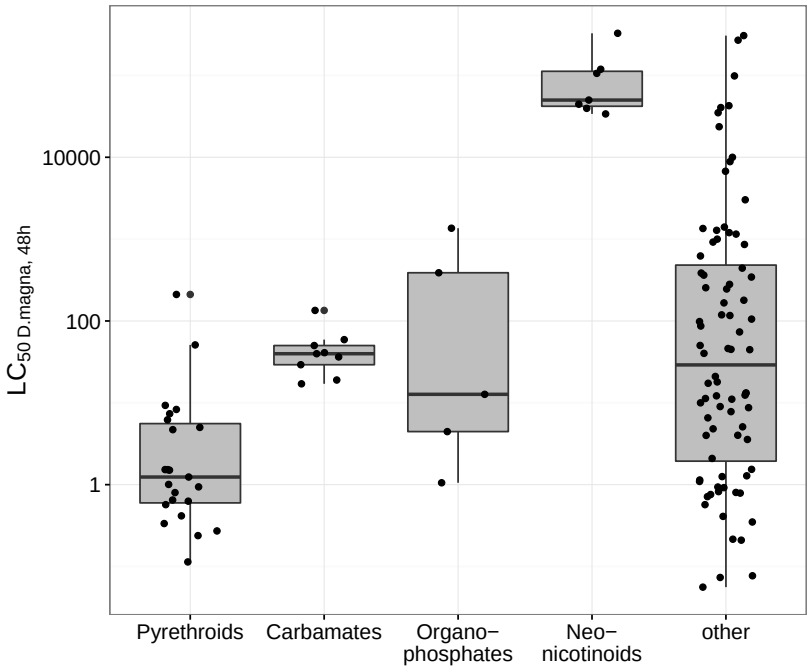

Figure 2: Toxicity of different pesticide groups. LC_{50} values have been retrieved from EPA ECOTOX database, chemical groups from the Compendium of Pesticide Common Names (Wood 2016)

4.5. Querying partitioning coefficients

Some data sources contain also data on chemical properties that can be queried. Here we query for the `lc50` data the log $P_{oct/wat}$ from the SRC PHYSPROP database to build a simple quantitative structure–activity relationship (QSAR) to predict toxicity.

```
R> pp_data <- pp_query(lc50$cas)
```

The database contains predicted and experimental values. Extracting log $P_{oct/wat}$ from the data object is slightly more complicated, because i) for some compounds no data could be found and ii) the data-object has a more complex structure (a data frame within a list).

```
R> lc50$logp <- sapply(pp_data, function(y) {
+    if (length(y) == 1 && is.na(y))
+      return(NA)
+    y$prop$value[y$prop$variable == 'Log P (octanol-water)']
+  })
```

We opted for this more complex approach, because the information available is very diverse and we cannot provide an extractor function for each purpose. Moreover, it gives users full control over how to organize their data. Nevertheless, we provide in the documentation of each function examples on how to extract more complicated parts of the data. The resulting data and model is displayed in Figure 3.

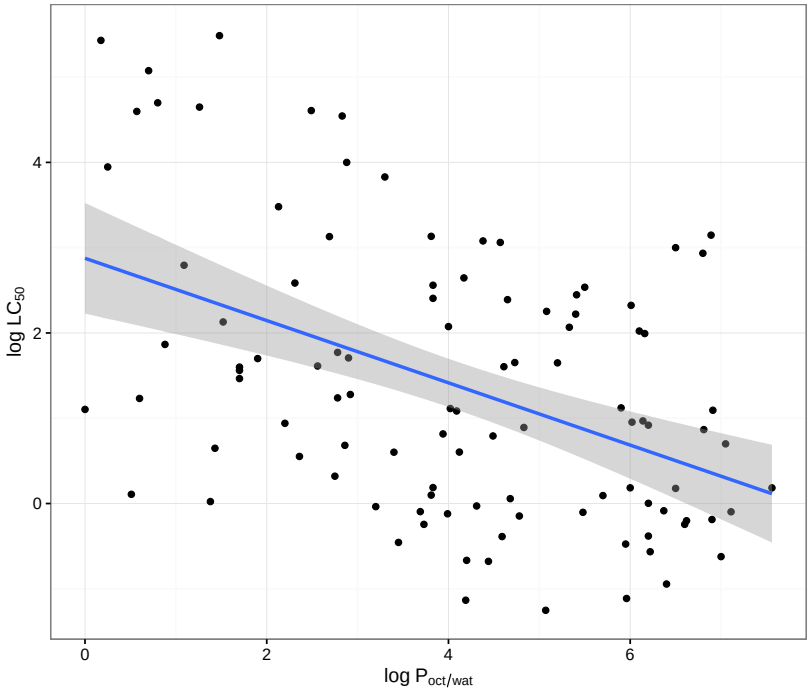

Figure 3: Simple QSAR for predicting log LC_{50} of pesticides by log P. Log P values have been retrieved from SRC Physprop database (97 experimental data, 9 estimated data and 18 substances without data). Blue line indicates the regression model ($\log LC_{50} = 2.88 - 0.37 \log P$, RMSE = 1.45).

4.6. Legal information

Legal information is particularly of interest if concentrations exceed national thresholds. In the European Union (EU) the Water Framework Directive (WFD) defines Environmental Quality Standards (EQS). Similarly, in the U.S. and Canadian EPA and the WHO defines Quality Standards. Information on these standards can be queried with **webchem** from the PAN Pesticide Database (using `pan_query()`) and from ETOX (using `etox_targets()`).

In this example we search for the minimum EQS for the EU for the compounds in the `jagst` data set, join these with measureds concentrations and check if there have been any ex-

ceedances.

We re-use the above queried ETOX-IDs to get further information from ETOX, namely the MAC-EQS:

```
R> eqs <- etox_targets(ids$etoxid)
R> ids$mac <- sapply(eqs, function(y){
+    if (length(y) == 1 && is.na(y)) {
+      return(NA)
+    } else {
+      res <- y$res
+      min(res[res$Country_or_Region == 'EEC / EU' &
+                res$Designation == 'MAC-EQS', 'Value_Target_LR'])
+    }
+  })
```

Again, the returned information is humongous and we encourage the users to study the returned objects and description of the data source. Here the column `Designation` defines the type of EQS and `Value_Target_LR` contains the value. Unfortunately, we found MAC-EQS values only for 5 substances:

```
R> (mac <- with(ids, ids[!is.na(mac) & is.finite(mac),
+                         c('etoxid', 'query', 'mac')]))
```

```
   etoxid       query    mac
4    8397     Atrazin  2.000
5    7240      Benzol 50.000
11   8836     Irgarol  0.016
12   7442 Isoproturon  1.000
29   8756   Terbutryn  0.034
```

The `get_etoxid()` function used to search ETOX-IDs returns also the original substance name (`query`), so that we can easily join the table with MAC values with the measurements table :

```
R> jagst_eqs <- merge(jagst, mac, by.x = 'substance', by.y = 'query')
R> head(jagst_eqs)
```

```
  substance       date  value qual etoxid mac
1   Atrazin 2013-09-10 0.0068    =   8397   2
2   Atrazin 2013-10-08 0.0072    =   8397   2
3   Atrazin 2013-03-26 0.0040    =   8397   2
4   Atrazin 2013-04-23 0.0048    =   8397   2
5   Atrazin 2013-11-05 0.0036    =   8397   2
6   Atrazin 2013-07-16 0.0052    =   8397   2
```

Finally, we can compare the measured value with the MAC, which reveals that there have been no exceedances of these 5 compounds.

4.7. Utility functions

Furthermore, **webchem** provides also basic functions to check identifiers that can be used for data quality assessment. The functions either use simple formatting rules,

```
R> is.inchikey('BQJCRHHNABKAKU-KBQPJGBKS-AN')

Hyphens not at position 15 and 26.

[1] FALSE

R> is.cas('64-17-6')

Checksum is not correct! 5 vs. 6

[1] FALSE
```

or web resources like ChemSpider

```
R> is.inchikey('BQJCRHHNABKAKU-KBQPJGBKSA-5',
+    type = 'chemspider')

[1] FALSE
```

5. Discussion

5.1. Related software

Within the R ecosystem, there are only few similar projects: **rpubchem** (Guha 2014) provides an interface PubChem. Similarly, **ChemmineR** (Cao *et al.* 2008), a mature chemo-informatics package, also provides an interface to Pubchem. **webchem** does not provide any chemo-informatic functionality, but integrates access to many data sources. **WikidataR** (Keyes and Graul 2016) provides an interface to wikidata that could be used to retrieve chemical data from Wikipedia. However, it does not provide predefined methods for chemical data like **webchem**. Within the Python ecosystem the libraries **PubChempy** (Swain 2015b), **ChemSpiPy** (Swain 2015a) and **CIRpy** (Swain 2016) are available for similar tasks as those outlined here. **webchem** is not specialized and tries to integrate many data sources and for some of these it provides a unique programmatic interface. The Chemical Translation Service (Wohlgemuth *et al.* 2010), which is also one of the sources that can be queried, allows batch conversion of chemical identifiers. However, it does not provide access to other data (experimental, modeled or legal data).

5.2. Open Science

An increasing number of scientific data is becoming publicly available (Gewin 2016; Reichman *et al.* 2011; O'Boyle *et al.* 2011), either in public data repositories or as supplement to publications. To be usable for other researchers chemical compounds should be properly identified,

not only by chemical names but also with accompanying identifiers like InChIKey, SMILES and authority-assigned identifiers. **webchem** provides an easy way to create such meta tables as shown in Table 1 and facilitates chemical data availability to researchers. However, good quality of data is crucial for every analysis (Stieger *et al.* 2014) and additional effort and methods are needed to validate data quality.

5.3. Further development

We have outlined only a few use cases that will likely be useful for many researchers. Given the huge amount of publicly available information, many other possibilities can be envisioned. **webchem** is currently under active development and several other data sources have not been implemented yet but may be in the future. GitHub makes contributing easy and we strongly encourage contribution to the package. Moreover, comments, feedback and feature requests are highly welcome.

6. Conclusions

Researchers need to have easy access to global knowledge on chemicals. **webchem** can save *"hundreds of working hours"* gathering this knowledge (Münch and Galizia 2016), so that researchers can focus on other tasks.

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Affiliation:

Eduard Szöcs
Institute for Environmental Sciences
Universität Koblenz-Landau
Fortstraße 7
76829 Landau, Germany
E-mail: szoecs@uni-landau.de
URL: https://edild.github.io

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