

```
devtools::install_github("NIVANorge/chemspiderapi")
```

Writing (tidyverse-friendly) packages

A three-course menu
with **devtools**
and friends*



Who am I?

- Raoul Wolf
- Biologist
- useR! since 2013
- Post Doc at the Norwegian Institute for Water Research (NIVA)



Today's Menu

1. Before writing a package



2. While writing a package*



3. After writing a package

Before writing a package

Why bother writing a package?!

Excursion into chemistry



Main page
Contents
Featured content
Current events
Random article
Donate to Wikipedia
Wikipedia store

Interaction

Help
About Wikipedia
Community portal
Recent changes
Contact page

Tools

What links here
Related changes
Upload file
Special pages
Permanent link
Page information
Wikidata item
Cite this page

Print/export

Create a book
Download as PDF

Not logged in [Talk](#) [Contributions](#) [Create account](#) [Log in](#)

Article [Talk](#)

[Read](#)

[View source](#)

[View history](#)



Caffeine

From Wikipedia, the free encyclopedia

This article is about the stimulant drug. For other uses, see [Caffeine \(disambiguation\)](#).

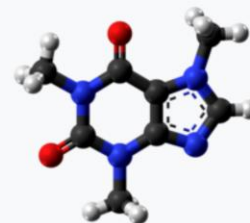
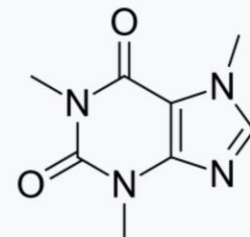
Caffeine is a **central nervous system (CNS) stimulant** of the **methylxanthine class**.^[10] It is the world's most widely consumed **psychoactive drug**. Unlike many other psychoactive substances, it is legal and unregulated in nearly all parts of the world. There are several known **mechanisms of action** to explain the effects of caffeine. The most prominent is that it reversibly blocks the action of **adenosine** on its receptor and consequently prevents the onset of drowsiness induced by adenosine. Caffeine also stimulates certain portions of the **autonomic nervous system**.

Caffeine is a bitter, white crystalline **purine**, a **methylxanthine alkaloid**, and is chemically related to the **adenine** and **guanine** bases of **deoxyribonucleic acid** (DNA) and **ribonucleic acid** (RNA). It is found in the seeds, nuts, or leaves of a number of plants native to Africa, East Asia and South America,^[11] and helps to protect them against predator insects and to prevent germination of nearby seeds.^[12] The most well-known source of caffeine is the **coffee bean**, a **misnomer** for the seed of *Coffea* plants. **Beverages** containing caffeine are ingested to relieve or prevent drowsiness and to improve performance. To make these drinks, caffeine is extracted by **steeping** the plant product in water, a process called **infusion**. Caffeine-containing drinks, such as **coffee**, **tea**, and **cola**, are very popular; as of 2014, 85% of American adults consumed some form of caffeine daily, consuming 164 mg on average.^[13]

Caffeine can have both positive and negative health effects. It can treat and prevent the premature infant breathing disorders **bronchopulmonary dysplasia** of prematurity and **apnea of prematurity**. **Caffeine citrate** is on the **WHO Model List of Essential Medicines**.^[14] It may confer a modest protective effect against some diseases,^[15] including **Parkinson's disease**.^[16] Some people experience **sleep disruption** or anxiety if they consume caffeine, but others show little disturbance. Evidence of a risk during pregnancy is equivocal; some authorities recommend that pregnant women limit consumption to the equivalent of two cups of coffee per day or less.^{[17][18]} Caffeine can produce a mild form of **drug dependence** – associated with **withdrawal symptoms** such as sleepiness, headache, and irritability – when an individual stops using caffeine after repeated daily intake.^{[1][3][5]} **Tolerance** to the autonomic effects of increased blood pressure and heart rate, and increased urine output, develops with chronic use (i.e., these symptoms become less pronounced or do not occur following consistent use).^[19]

Caffeine is classified by the US **Food and Drug Administration** as "**generally recognized as safe**" (GRAS). Toxic doses, over 10 grams per day for an adult, are much higher than the typical dose of under 500 milligrams per day. A cup of coffee contains 80–175 mg of caffeine, depending on what "bean" (seed) is used and how it is prepared (e.g., **drip**, **percolation**, or **espresso**). Thus it requires roughly 50–100 ordinary cups of coffee to reach the toxic dose. However, pure powdered caffeine, which is available as a **dietary supplement**, can be lethal in tablespoon-sized amounts.

Caffeine



Clinical data

Pronunciation /ˈkæf.i.n./, ˈkæf.i.n/
Synonyms Cupressine

Excursion into chemistry

| Identifiers | |
|-------------------------------------|---|
| IUPAC name | [hide] 1,3,7-Trimethylpurine-2,6-dione |
| CAS Number | 58-08-2 ✓ |
| PubChem CID | 2519 ✓ |
| IUPHAR/BPS | 407 ✓ |
| DrugBank | DB00201 ✓ |
| ChemSpider | 2424 ✓ |
| UNII | 3G6A5W338E ✓ |
| KEGG | D00528 ✓ |
| ChEBI | CHEBI:27732 ✓ |
| ChEMBL | CHEMBL113 ✓ |
| PDB ligand | CFF (PDB ✓, RCSB PDB ✓) |
| ECHA InfoCard | 100.000.329 ✓ |
| Chemical and physical data | |
| Formula | C ₈ H ₁₀ N ₄ O ₂ |
| Molar mass | 194.19 g/mol |
| 3D model (JSmol) | Interactive image |
| Density | 1.23 g/cm ³ |
| Melting point | 235 to 238 °C (455 to 460 °F) (anhydrous) ^{[8][9]} |
| SMILES | [hide] <chem>CN1C=NC2=C1C(=O)N(C(=O)N2C)C</chem> |
| InChI | [hide] InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/14h,1-3H3 |
| Key | Key:RYYVLZVUVIJVGH-UHFFFAOYSA-N ✓ |
| See also: data page | |

InChIKey

RYYVLZVUVIJVGH-UHFFFAOYSA-N

Before writing a package

The screenshot shows the ChemSpider website interface. The browser's address bar displays <https://www.chemspider.com>. The navigation bar includes links for Home, About us, Web APIs (circled in orange), Help, and Sign in. The ChemSpider logo and tagline 'Search and share chemistry' are prominent. A search bar is located on the right side of the header. Below the header, there are tabs for Simple, Structure, Advanced, and History. The main content area features a large search box with the text 'Search ChemSpider' and a search button. Below this, there is a section titled 'Search ChemSpider' with a description: 'Matches any text strings used to describe a molecule.' and a search input field. Below the search input, there is a link to 'Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID'. The page is divided into four columns: 'What is ChemSpider?', 'Search by chemical names', 'Search by chemical structure', and 'Find important data'. Each column contains a list of features or search capabilities. At the bottom, there is a 'Blog' section with a 'Subscribe' button and a large graphic showing '68 Million'.

File Edit View History Bookmarks Tools Help

ChemSpider | Search and share X Traffic - NIVANorge/chemspide X Switch to new chemspider Api X ChemSpider API direct docum X +

← → ⓘ https://www.chemspider.com ... ☆ ↻ 🏠 ⬇ 📄 🔍 Search

Home About us **Web APIs** Help Sign in

ChemSpider
Search and share chemistry

Search ChemSpider 🔍

Simple Structure Advanced History

Search ChemSpider

Matches any text strings used to describe a molecule.

Search 🔍

Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID ⓘ

Advertisement

| What is ChemSpider? | Search by chemical names | Search by chemical structure | Find important data |
|---|--|---|--|
| <p><i>ChemSpider</i> is a free chemical structure database providing fast text and structure search access to over 67 million structures from hundreds of data sources.</p> | <ul style="list-style-type: none">• Systematic names• Synonyms• Trade names• Database identifiers | <ul style="list-style-type: none">• Create structure-based queries• Draw structures in the web page• Use structure files from your computer | <ul style="list-style-type: none">• Literature references• Physical properties• Interactive spectra• Chemical suppliers |

What is ChemSpider?

ChemSpider is a free chemical structure database providing fast text and structure search access to over 67 million structures from hundreds of data sources.

Search by chemical names

- Systematic names
- Synonyms
- Trade names
- Database identifiers

Search by chemical structure

- Create structure-based queries
- Draw structures in the web page
- Use structure files from your computer

Find important data

- Literature references
- Physical properties
- Interactive spectra
- Chemical suppliers

Blog

Subscribe

Royal Society of Chemistry Renews Partnership with ACD/Labs

68 Million

Before writing a package

The screenshot shows a web browser window with the CRAN page for the 'webchem' package. The browser's address bar shows the URL <https://cran.r-project.org/web/packages/webchem/>. The page title is 'webchem: Chemical Information from the Web'. The main content area lists package details: Version (0.4.0), Depends (R (≥ 3.0)), Imports (xml2, http, rvest, RCurl, jsonlite, stringr, methods), Suggests (testthat, rcdk), Published (2018-04-07), Author (Eduard Szöcs [aut, cre], Daniel Muench [ctb], Johannes Ranke [ctb], Eric Scott [ctb], Jan Stanstrup [ctb], Robert Allaway [ctb]), Maintainer (Eduard Szöcs <eduardsoecs at gmail.com>), BugReports (<https://github.com/ropensci/webchem/issues>), License (MIT + file LICENSE), URL (<https://github.com/ropensci/webchem>), NeedsCompilation (no), Citation ([webchem citation info](#)), Materials ([NEWS](#)), In views ([ChemPhys](#)), and CRAN checks ([webchem results](#)). Below this, the 'Downloads' section lists the Reference manual ([webchem.pdf](#)), Package source ([webchem 0.4.0.tar.gz](#)), Windows binaries (r-devel: [webchem 0.4.0.zip](#), r-release: [webchem 0.4.0.zip](#), r-oldrel: [webchem 0.4.0.zip](#)), OS X binaries (r-release: [webchem 0.4.0.tgz](#), r-oldrel: [webchem 0.4.0.tgz](#)), and Old sources ([webchem archive](#)). The 'Linking' section at the bottom states: 'Please use the canonical form <https://CRAN.R-project.org/package=webchem> to link to this page.'

File Edit View History Bookmarks Tools Help

ChemSpider | Search and share X NIVANorge/chemspideR: Conv X CRAN - Package webchem X Switch to new chemspideR Api X ChemSpider API direct docum X +

← → ⓘ <https://cran.r-project.org/web/packages/webchem/> ... ☆ ↻ 🏠 ⬇️ 🔍 Search

webchem: Chemical Information from the Web

Chemical information from around the web. This package interacts with a suite of web APIs for chemical information.

Version: 0.4.0
Depends: R (≥ 3.0)
Imports: [xml2](#), [http](#), [rvest](#), [RCurl](#), [jsonlite](#), [stringr](#), methods
Suggests: [testthat](#), [rdck](#)
Published: 2018-04-07
Author: Eduard Szöcs [aut, cre], Daniel Muench [ctb], Johannes Ranke [ctb], Eric Scott [ctb], Jan Stanstrup [ctb], Robert Allaway [ctb]
Maintainer: Eduard Szöcs <eduardsoecs at gmail.com>
BugReports: <https://github.com/ropensci/webchem/issues>
License: [MIT](#) + file [LICENSE](#)
URL: <https://github.com/ropensci/webchem>
NeedsCompilation: no
Citation: [webchem citation info](#)
Materials: [NEWS](#)
In views: [ChemPhys](#)
CRAN checks: [webchem results](#)

Downloads:

Reference manual: [webchem.pdf](#)
Package source: [webchem 0.4.0.tar.gz](#)
Windows binaries: r-devel: [webchem 0.4.0.zip](#), r-release: [webchem 0.4.0.zip](#), r-oldrel: [webchem 0.4.0.zip](#)
OS X binaries: r-release: [webchem 0.4.0.tgz](#), r-oldrel: [webchem 0.4.0.tgz](#)
Old sources: [webchem archive](#)

Linking:

Please use the canonical form <https://CRAN.R-project.org/package=webchem> to link to this page.



Before writing a package

File Edit View History Bookmarks Tools Help

RSC Developer Portal | Chem: X NIVANorge/chemspideR: Cor: X CRAN - Package webchem X Switch to new chemspideR: A: X ChemSpider API direct docum: X NIVANorge/chemspideR: Cor: X The ChemSpider APIs service has X

link.rsc.org/rsp/m/xSq8Cm8ovjN8-Elm0eYB3Sey61zutqNIUUaMcy14sQ

Online Version Follow us: f t in y



The old ChemSpider APIs service is being turned off on 30 November 2018

As you know, we have migrated the ChemSpider API functionality to a new API platform. On 1 December, you will no longer be able to access the old ChemSpider API service.


Register to access the new APIs platform

If you want to access the new APIs please [register with our new portal](#).

If you have any questions about the migration or if you'd would be willing to talk to us about your current use of APIs please [get in touch](#).

Register for access

Best wishes
Royal Society of Chemistry



www.rsc.org
Registered charity number: 207690

You have been sent this message because you have registered for access to ChemSpider. If you feel that you have received this in error, please contact publishing@rsc.org.

Before writing a package

The screenshot shows a web browser window with the URL <https://developer.rsc.org/compounds-v1/apis>. The page is titled "ChemSpider Compound APIs" and describes the service as a way to "Interrogate and access chemical data, powered by the Royal Society of Chemistry's ChemSpider database."

The page features a "FILTERING" section with a table of API endpoints:

| METHOD | DESCRIPTION |
|---|--|
| POST https://api.rsc.org/compounds/v1/filter/element | filter-element-post Submit an array called 'includeElements' of up to 15 elements and an array called 'excludeElements' of up to 100 elements via POST. This endpoint will... |
| POST https://api.rsc.org/compounds/v1/filter/formula/batch | filter-formula-batch-post Submit an array of up to 100 formulas via POST. You can optionally supply dataSources as a JSON-formatted array of up to 20 strings, representing the... |
| GET https://api.rsc.org/compounds/v1/filter/formula/batch/{queryId}/results | filter-formula-batch-queryId-results-get Call this endpoint with a queryId returned from the /filter/formula/batch filter query. The queryId supplied must return 'Complete' when submitted to ... |
| GET https://api.rsc.org/compounds/v1/filter/formula/batch/{queryId}/status | filter-formula-batch-queryId-status-get Call this endpoint with a queryId returned from the /filter/formula/batch filter query. If successful, returns a JSON object. This object contains 's... |
| POST https://api.rsc.org/compounds/v1/filter/formula | filter-formula-post Submit formula as a string via POST. You can optionally supply dataSources as a JSON-formatted array of up to 20 strings, representing the data sourc... |

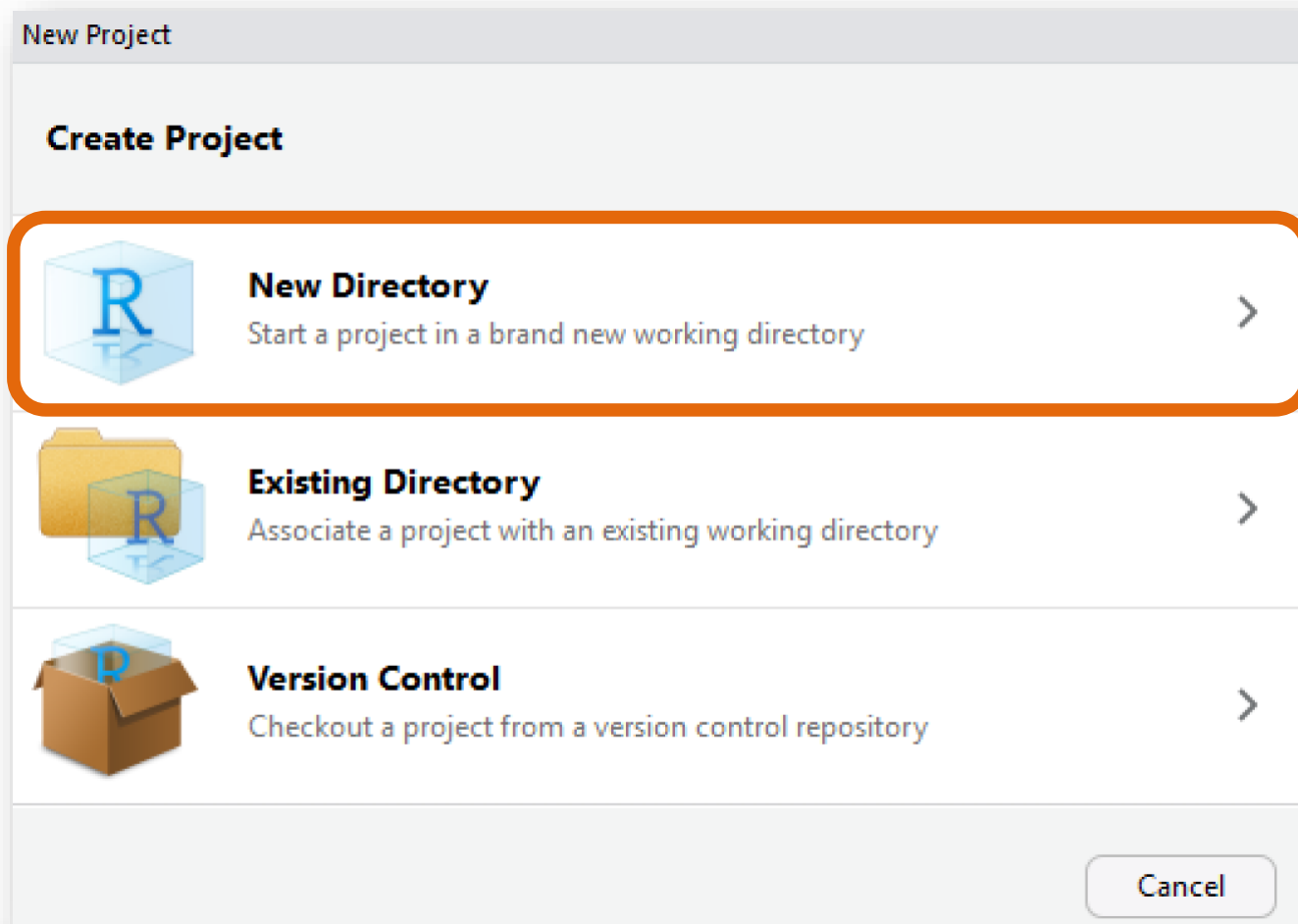
At the bottom of the page, there is a footer with the Royal Society of Chemistry logo, copyright information (© Royal Society of Chemistry 2018, Registered charity number: 207890), and links for Privacy Policy, Terms & Use, and Contact.

Before writing a package

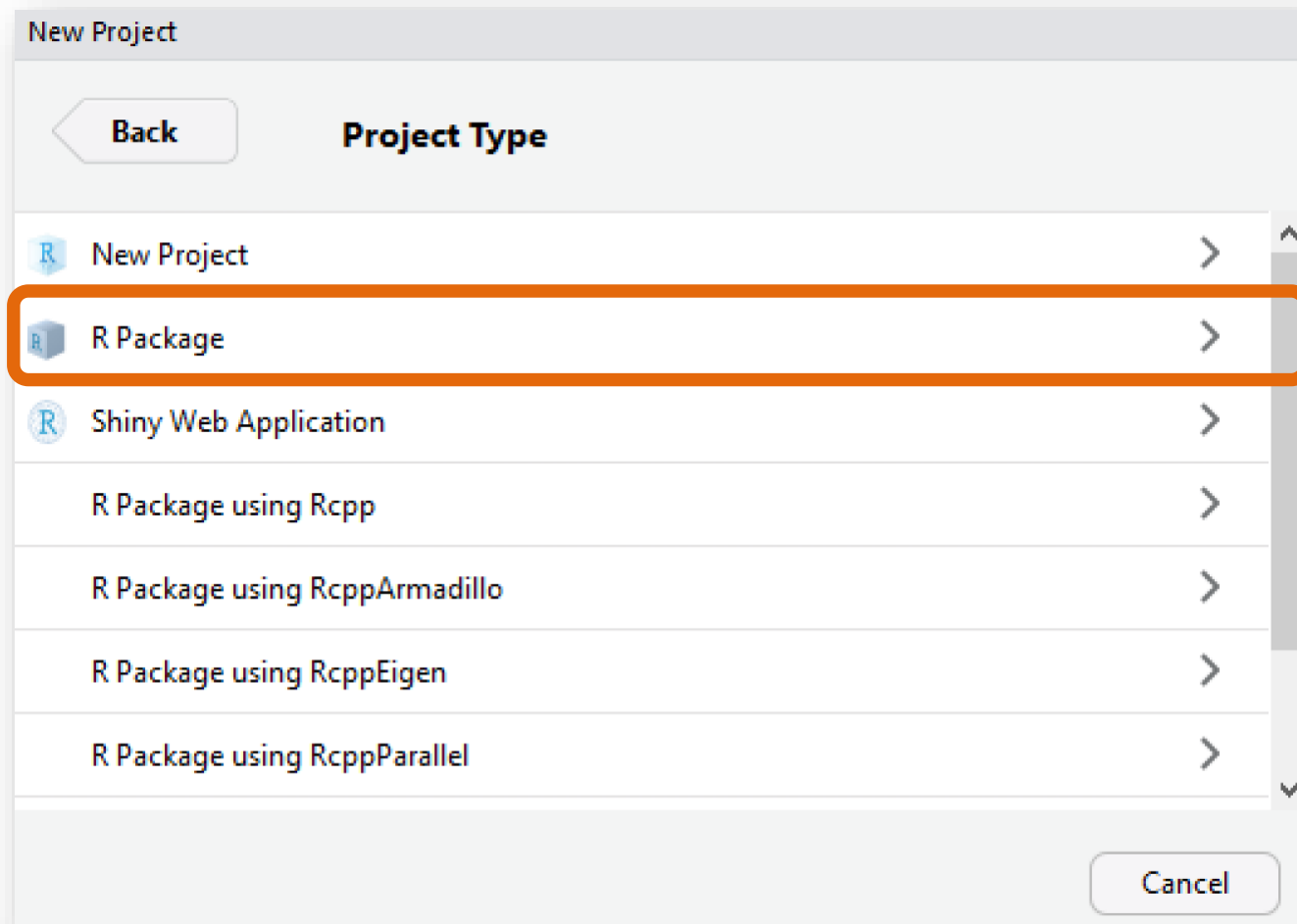
Things to consider / constraints

- Useable for base R and `tidyverse` styles
- As little (recursive) dependencies as possible
- Know your audience!

While writing a package



While writing a package



While writing a package

New Project

Create R Package

Back

Type: Package

Package name:

Create package based on source files:

Add...

Remove

Create project as subdirectory of:

C:/R/packages

Browse...

☐ Create a git repository ☐ Use packrat with this project

☐ Open in new session

Create Project Cancel

While writing a package

The screenshot displays the RStudio interface for a package named 'atestpackage'. The main editor window shows a file named 'hello.R' with the following content:

```
1 # Hello, world!
2 #
3 # This is an example function named 'hello'
4 # which prints 'Hello, world!'.
5 #
6 # You can learn more about package authoring with RStudio at:
7 #
8 # http://r-pkgs.had.co.nz/
9 #
10 # Some useful keyboard shortcuts for package authoring:
11 #
12 #   Build and Reload Package: 'Ctrl + Shift + B'
13 #   Check Package:           'Ctrl + Shift + E'
14 #   Test Package:             'Ctrl + Shift + T'
15 #
16 hello <- function() {
17   print("Hello, world!")
18 }
19
```

The console window at the bottom shows the R version and copyright information:

```
R version 3.5.1 (2018-07-02) -- "Feather Spray"
Copyright (C) 2018 The R Foundation for Statistical Computing
Platform: x86_64-w64-mingw32/x64 (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> |
```

The Environment pane on the right shows the 'Global Environment' with the message 'Environment is empty'. The Files pane on the right shows the directory structure of the package:

| Name | Size | Modified |
|--------------------|-------|----------------------|
| .. | | |
| .gitignore | 44 B | Nov 7, 2018, 9:51 AM |
| .Rbuildignore | 30 B | Nov 7, 2018, 9:51 AM |
| atestpackage.Rproj | 376 B | Nov 7, 2018, 9:51 AM |
| DESCRIPTION | 383 B | Nov 7, 2018, 9:51 AM |
| man | | |
| NAMESPACE | 32 B | Nov 7, 2018, 9:51 AM |
| R | | |

While writing a package

Necessary files:

- DESCRIPTION
- LICENSE: `usethis::use_mit_license("Your Name")`
- NAMESPACE
- README.md: `usethis::use_readme_rmd()`

While writing a package

devtools::

| | | |
|---|-------------------------------|---|
| 1 | create() | <i>RStudio</i> |
| 2 | | <code>usethis::use_mit_license()</code> |
| 3 | <code>use_readme_rmd()</code> | <code>usethis::use_readme_rmd()</code> |
| 4 | <code>document()</code> | <code>roxygen2::roxygenize()</code> |
| 5 | <code>load_all()</code> | <code>pkgload::load_all()</code> |
| 6 | <code>check()</code> | <code>rcmdcheck::rcmdcheck()</code> |
| 7 | <code>build()</code> | <code>pkgbuild::build()</code> |
| 8 | <code>install()</code> | |

While writing a package

What makes a function/package tidyverse friendly?

- First function argument is the input data
- Easily* applicable in `purrr::map_*()` functions
- `typeof()` output needs to be consistent

While writing a package

Let's look at my **chemspiderapi**
package in RStudio!

While writing a package

Example:

One line of functionalities

- `chemspiderapi::post_inchikey()`
- `chemspiderapi::get_queryId_status()`
- `chemspiderapi::get_queryId_result()`
- `chemspiderapi::get_recordId_details()`

After writing a package

Where is the *testing*?

After writing a package

Publishing!

```
devtools::install_github("NIVANorge/chemspiderapi")
```

After writing a package

Maintenance...

```
devtools::install_github("NIVANorge/chemspiderapi")
```

Writing (tidyverse-friendly) packages

A three-course menu
with **devtools**
and friends*

