Package: Ropenbabel (via r-universe)

November 24, 2026

Title Open Babel cheminformatics C++ library as an R package

Description Provides version 3.2.1 of the Open Babel C++ library, built as a static library, together with its headers and data files. Intended for developers of other R packages (such as ChemmineOB) who want to link against Open Babel without requiring a system installation. Use Ropenbabel::pkgconfig() in Makevars.

Version 0.99.0

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LinkingTo RcppEigen

Suggests knitr, rmarkdown, BiocStyle

VignetteBuilder knitr

SystemRequirements cmake (>= 3.12), GNU make, C++17, cairo (optional, for PNG output), pkg-config (optional)

biocViews Cheminformatics, Infrastructure

URL https://github.com/girke-lab/Ropenbabel

BugReports https://github.com/girke-lab/Ropenbabel/issues

Config/pak/sysreqs libcairo2-dev cmake make pkg-config

Repository https://biocstaging.r-universe.dev

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`Ropenbabel-package` *Open Babel C++ library for R packages*

Description

Ropenbabel builds the Open Babel cheminformatics library from bundled sources as a static library when the package is installed, and installs its headers and data files. Other packages, such as **ChemmineOB**, link to it with the flags from `pkgconfig`, so they need no system installation of Open Babel.

See Also

`pkgconfig`, `vignette("Ropenbabel")`

`pkgconfig` *Build flags, data directory and version of the bundled Open Babel*

Description

Helpers for packages that link to the static Open Babel library shipped in **Ropenbabel**.

Usage

```
pkgconfig(opt = c("PKG_LIBS", "PKG_CPPFLAGS"))
dataDir()
obVersion()
```

Arguments

`opt`	Which flags to print: `"PKG_CPPFLAGS"` (include path) or `"PKG_LIBS"` (static libraries plus any system libraries, such as Cairo, that they were built against).

Details

`pkgconfig` is meant to be called from a client package's '`src/Makevars`' (or '`src/Makevars.win`'):

```
RSCRIPT = "$(R_HOME)/bin/Rscript"
PKG_CPPFLAGS = $(shell $(RSCRIPT) -e "Ropenbabel::pkgconfig('PKG_CPPFLAGS')")
PKG_LIBS     = $(shell $(RSCRIPT) -e "Ropenbabel::pkgconfig('PKG_LIBS')")
```

together with `LinkingTo: Ropenbabel` and `Imports: Ropenbabel` in '`DESCRIPTION`'.

Open Babel reads force fields, atom types and other data files from the directory named by the `BABEL_DATADIR` environment variable. **Ropenbabel** sets it to `dataDir()` when loaded, unless it is already set.

Value

pkgconfig prints the flags with cat and returns NULL invisibly. dataDir returns the path of the Open Babel data directory. obVersion returns the Open Babel version as a character string.

Examples

```
pkgconfig("PKG_CPPFLAGS")
pkgconfig("PKG_LIBS")
dataDir()
obVersion()
```

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