

ChemmineDrugs

June 12, 2024

ChemmineDrugs

Chemmine Drugs

Description

This package contains a pre-built SQLite database of the DrugBank data set. The DUD database can also be downloaded using the `DUD()` function in ChemmineR. It is no longer included in this package because of its large size (1.8GB zipped)

These databases can be used with functions in the ChemmineR package to perform compound searches and also to retrieve pre-computed features for each compound.

Author(s)

Kevin Horan

See Also

[ChemmineR](#)

Examples

```
library(ChemmineDrugs)
## list included databases
dir(system.file("extdata", package="ChemmineDrugs"))

## Not run:
library(ChemmineR)
conn = DrugBank()

## End(Not run)
```

Index

ChemmineDrugs, [1](#)

ChemmineR, [1](#)