Package 'LipinskiFilters'

May 7, 2026

Title Computes and Visualize Lipinski's Parameters

Version 1.0.1

Description This computes Lipinski Rule of Five parameters and offers visualization for drug discovery. It analyzes molecular properties like molecular weight, hydrogen bond donors, acceptors, and ALogP, providing histograms and pass/fail status plots for efficient compound evaluation, aiding in drug development.

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Encoding UTF-8

RoxygenNote 7.2.3

Depends R (>= 3.6.0), cowplot, rcdk (>= 3.8.1), ggplot2

Imports itertools (>= 0.1-3), utils, knitr

VignetteBuilder knitr

NeedsCompilation no

Author Oche Ambrose George [aut, cre] (ORCID: <https://orcid.org/0000-0002-3979-6232>)

Maintainer Oche Ambrose George <ocheab1@gmail.com>

Repository CRAN

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Suggests rmarkdown

Contents

assess_drug_likeness *Assess drug-likeness*

Description

This function assesses the drug-likeness of molecules based on calculated molecular properties.

Usage

```
assess_drug_likeness(properties_df)
```

Arguments

properties_df	Data frame with molecular properties.

Value

Data frame with an additional column indicating whether each molecule is drug-like or not.

compute_properties *Compute molecular properties*

Description

This function computes molecular properties based on input molecules.

Usage

```
compute_properties(mols)
```

Arguments

mols	Molecules data.

Value

Data frame with calculated properties including Molecular Weight (MW), number of Hydrogen Bond Donors (nHBDon), number of Hydrogen Bond Acceptors (nHBAcc), Topological Polar Surface Area (TPSA), and ALogP.

create_lipinski_plots *Create Lipinski plots*

Description

This function creates plots illustrating the distribution of molecular properties and the pass/fail status of Lipinski's Rule of Five.

Usage

```
create_lipinski_plots(properties_df)
```

Arguments

properties_df	Data frame with molecular properties and pass/fail status.

Value

A grid of plots showing distributions and pass/fail status.

mols *Molecules read into R in sdf format*

Description

This object contains molecules read into R using the 'load.molecules' function

predict_oral_bioavailability *Predict oral bioavailability*

Description

This function predicts the oral bioavailability of molecules based on calculated molecular properties.

Usage

```
predict_oral_bioavailability(properties_df)
```

Arguments

properties_df	Data frame with molecular properties.

Value

Data frame with an additional column indicating whether each molecule has high or low oral bioavailability.

`test_lipinski_rule` *Test Lipinski's Rule of Five*

Description

This function tests Lipinski's Rule of Five based on calculated molecular properties.

Usage

```
test_lipinski_rule(properties_df)
```

Arguments

`properties_df`	Data frame with molecular properties.

Value

A vector indicating whether each molecule passes or fails Lipinski's Rule of Five.

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