# Package: LipinskiFilters (via r-universe)

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**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

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**Suggests** rmarkdown

**Repository** https://cran.r-universe.dev

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`assess_drug_likeness` *Assess drug-likeness*

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## 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.

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`compute_properties` *Compute molecular properties*

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## 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.

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

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## 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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