

# Package: LipinskiFilters (via r-universe)

June 11, 2024

**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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**Date/Publication** 2024-03-11 15:20:05 UTC

**Suggests** rmarkdown

**Repository** <https://ocheab.r-universe.dev>

**RemoteUrl** <https://github.com/cran/LipinskiFilters>

**RemoteRef** HEAD

**RemoteSha** 6ad4489c6dd984a0cf5620aa1e56ea1ea30548ed

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assess_drug_likeness	<i>Assess drug-likeness</i>
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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	<i>Compute molecular properties</i>
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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.

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create\_lipinski\_plots *Create Lipinski plots*

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**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.

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mols *Molecules read into R in sdf format*

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**Description**

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

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predict\_oral\_bioavailability  
*Predict oral bioavailability*

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**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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