Package: MS2Quant (via r-universe)

November 3, 2024

Title Ionization efficiency prediction and quantification of unidentified chemicals

Version 1.1.0

Description MS2Quant harvests pre-trained xgbTree algorithm-based ionization efficiency prediction model. Using strucutral information (SMILES) or predicted fingerprints calculated with SIRIUS+CSI_FingerID software, ionization efficiency can be predicted. If calibrants have been measured together with suspects subject to quantification, predicted ionization efficiencies can be converted into measurement-specific response factors and concentration of unknown chemcals can be estimated.

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Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.2.3

LazyData true

Imports enviPat, rJava, rlist, rcdklibs, rcdk, xgboost, ggplot2, tidyr, dplyr, readr, tibble, xfun, stringr

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

RemoteUrl https://github.com/drewszabo/MS2Quant

RemoteRef main

RemoteSha 46e0c77ef4961a29a73a388105eeb28e33839630

Contents

isotopedistribution *Isotope distribution*

Description

This function calculates isotopic abundance for a chemical based on SMILES notation. This number can later be used as a coefficient to multiply the area corresponding to a monoisotopic ion.

Usage

```
isotopedistribution(smiles)
```

Arguments

smiles	SMILES notation of the compound

Value

isotopic abundance coefficient

Examples

```
isotopedistribution("CN1C=NC2=C1C(=O)N(C(=O)N2C)C")
```

linear_regression *Linear regression*

Description

This function calculates the linear regression parameters from specified x and y values. Additionally, it checks the linearity based on residuals. In case there exists a residual with absolute value higher than 10, the highest value x-y point will be removed and new linear regression is generated without it. At least 5 datapoints have to remain.

Usage

```
linear_regression(y, x, remove_lowest_conc = FALSE)
```

Arguments

y	y-values of the data corresponding to x-values
x	x-values of the data

Value

linear regression parameters (slope and intercept) as a list

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