Package ‘MSbox’

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Title Mass Spectrometry Tools
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Author Yonghui Dong
Maintainer Yonghui Dong <yonghui.dong@gmail.com>
Description Common mass spectrometry tools described in John Roboz (2013) <doi:10.1201/b15436>. It allows checking element isotopes, calculating (isotope labelled) exact monoisotopic mass, m/z values and mass accuracy, and inspecting possible contaminant mass peaks, examining possible adducts in electrospray ionization (ESI) and matrix-assisted laser desorption ionization (MALDI) ion sources.
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Imports stringr, xml2, stats
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Description

calculate common adduct ions in positive or negative ion mode

Usage

```r
adduct(F, mode = c("+", "-"))
```

Arguments

- `F` : chemical formula, case insensitive
- `mode` : ionization mode, either positive '+' or negative '-'

Author(s)

Yonghui Dong

Examples

```r
adduct('C1H4', mode = '-')
adduct('C1H4', mode = '+')
```

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Description

check the possible contaminants

Usage

```r
contam(mz, ppm = 10, mode = c("+", "-"))
```

Arguments

- `mz` : suspected m/z value
- `ppm` : mass tolerance, default value = 10
- `mode` : ionization mode, either positive '+' or negative '-'
describe

Author(s)

Yonghui Dong

Examples

```r
contam(33.0335, ppm = 10, mode = '+')
contam(44.998, ppm = 10, mode = '-')
```

describe  Get the compound information

Description

get compound formula and structure from https://cactus.nci.nih.gov/chemical/structure

Usage

```r
describe(chem, representation = "formula", info = FALSE)
```

Arguments

chem, chemical name of the compound
representation, representation methods, formula is default
info, extra molecular information that users can query

Author(s)

Yonghui Dong

Examples

```r
describe('malic acid', "formula")
describe(c('malic acid', 'citric acid', 'tartaric acid'), "smiles")
```
**E_iso**  
*Element isotopes*

**Description**  
check element isotope information

**Usage**  
\[ E_{iso}(S) \]

**Arguments**  
\[ S \]  
element, can be element symbol (i.e. C) or full name (i.e. Carbon). Both Element symbol and full name are case insensitive.

**Author(s)**  
Yonghui Dong

**Examples**  
\[
E_{iso}('Na') \quad \# \text{ element symbol} \\
E_{iso}('nA') \quad \# \text{ element symbol, case insensitive} \\
E_{iso}('Carbon') \quad \# \text{ element full name} \\
E_{iso}('carBon') \quad \# \text{ element full name, case insensitive}
\]

**Iso_mass**  
*Isotope labelled molecular mass*

**Description**  
Calculate isotope labelled molecular mass

**Usage**  
\[ Iso\_mass(F, iso) \]

**Arguments**  
\[ F, \quad \text{chemical formula, case insensitive} \]
\[ iso, \quad \text{labelled elements, case insensitive} \]

**Author(s)**  
Yonghui Dong
### Iso_mz

**Examples**

```r
Iso_mz(F = 'C7H6O4', iso = '[13]C2[2]H3') # Two 13C and three 2H are labeled
```

---

**Description**

Calculate isotope labelled m/z

**Usage**

```r
Iso_mz(F, iso, z)
```

**Arguments**

- `F`: chemical formula, case insensitive
- `iso`: labelled elements, case insensitive
- `z`: charge

**Author(s)**

Yonghui Dong

**Examples**

```r
Iso_mz(F = 'C7H6O4', iso = '[13]C2[2]H3', z = -1) # Two 13C and three 2H are labeled
```

---

### mass

**Description**

Calculate accurate molecular mass

**Usage**

```r
mass(F)
```

**Arguments**

- `F`: chemical formula, case insensitive

**Author(s)**

Yonghui Dong
Examples

```
mass('C7H6O4')
mass('c7H6O4') # case insensitive
mass(c('K1', 'C5H8', 'nA20')) # vector input
```

---

\textit{mz}

\textit{accurate ion mass}

Description

calculate accurate ion mass

Usage

```
mz(m, z)
```

Arguments

- \textit{m} chemical formula of an ion, case insensitive
- \textit{z} charge

Author(s)

Yonghui Dong

Examples

```
mz('C7H7O4', z = 1)
mz('C1O6C11', z = -1)
mz('C1H7O4', z = 1) # case insensitive
mz(c('C7H7O4', 'Cl'), z = -1) # vector input
```

---

\textit{ppm}

\textit{mass accuracy}

Description

calculate the mass accuracy of measured m/z. lazy input allowed

Usage

```
ppm(m, t, lazy = TRUE)
```
what

Arguments

m measured m/z
t theoretical m/z
lazy if lazy input is allowed

Author(s)

Yonghui Dong

Examples

ppm(155.03383, 155.03388) # with m/z value
ppm(155.03383, .03388) # lazy input when the integer parts of m and t are the same
ppm(155.03384, mz('C7H7O4', z = 1)) # with ion formula

what search for m/z in from the idiom metabolomics database

Description

tentative metabolite identification based on m/z value search

Usage

what(mz, mode = NULL, ppm = 5)

Arguments

mz m/z values
mode ionization mode, either positive '+' or negative '-'
ppm mass tolerance, default value = 10

Author(s)

Yonghui Dong

Examples

what(133.014, ppm = 10, mode = '-')