Package 'MSbox'

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Type Package

Title Mass Spectrometry Tools

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Description Common mass spectrometry tools described in John Roboz (2013) <doi:10.1201/b15436>. It allows checking element isotopes, calculating (isotope labelled) exact monoisitopic 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.

Depends R (>= 2.0.0)

Imports stringr, xml2, magick

License GPL-2

URL https://github.com/YonghuiDong/MSbox

BugReports https://github.com/YonghuiDong/MSbox/issues/new

Encoding UTF-8

LazyData true

RoxygenNote 6.0.1

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`adduct` *Common adducts*

Description

calculate common adduct ions in positive or negative ion mode

Usage

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

Arguments

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

Examples

```
adduct('C1H4', mode = '-')
adduct('C1h4', mode = '+')
```

`contam` *Contaminants in MS*

Description

check the possible contaminants

Usage

```
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 '-'

Examples

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

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.

Examples

```
E_iso('Na') # element symbol
E_iso('nA') # element symbol, case insensitive
E_iso('Carbon') # element full name
E_iso('carBon') # element full name, case insensitive
```

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formula *Get compound formula and structure*

Description

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

Usage

```
formula(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

Examples

```
formula('malic acid')
```

Iso_mass *Isotope labelled molecular mass*

Description

Calculate isotope labelled molecular mass

Usage

```
Iso_mass(F, iso)
```

Arguments

F,	chemical formula, case insensitive
iso,	labelled elements, case insensitive

Examples

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

Iso_mz *Isotope labelled molecular mass*

Description

Calculate isotope labelled m/z

Usage

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

Arguments

F,	chemical formula, case insensitive
iso,	labelled elements, case insensitive
z	charge

Examples

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

mass *molecular mass*

Description

calculate accurate molecular mass

Usage

```
mass(F)
```

Arguments

F	chemical formula, case insensitive

Examples

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

mz *accurate ion mass*

Description

calculate accurate ion mass

Usage

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

Arguments

m	chemical formula of an ion, case insensitive
z	charge

Examples

```
mz('C7H7O4', z = 1)
mz('C10H6Cl1', z = -1)
mz('C7h7O4', z = 1) # case insensitive
mz(c('C7H7O4', 'c1'), z = -1) # vector input
```

ppm *mass accuracy*

Description

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

Usage

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

Arguments

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

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
```

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