# Package 'MSbox'

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**Type** Package

**Title** Mass Spectrometry Tools

**Version** 1.2.1

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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 (>= 3.5.0)

**Imports** stringr, xml2, stats

**License** GPL-2

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

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

**Encoding** UTF-8

**LazyData** true

**RoxygenNote** 6.1.1

**NeedsCompilation** no

**Repository** CRAN

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## R topics documented:

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`adduct` *Common adducts*

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## 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 '-' |

## Author(s)

Yonghui Dong

## Examples

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

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`contam` *Contaminants in MS*

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## 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 '-' |

### Author(s)

Yonghui Dong

### Examples

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

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## describe *Get the compound information*

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### Description

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

### Usage

```
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

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

## 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 |

### Author(s)

Yonghui Dong

### Examples

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

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`Iso_mz` *Isotope labelled molecular mass*

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### 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 |

### Author(s)

Yonghui Dong

### Examples

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

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`mass` *molecular mass*

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### Description

calculate accurate molecular mass

### Usage

```
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
```

---

## mz *accurate ion mass*

---

### Description

calculate accurate ion mass

### Usage

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

### Arguments

| | |
|---|---|
| m | chemical formula of an ion, case insensitive |
| z | charge |

### Author(s)

Yonghui Dong

### Examples

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

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## 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 |

### 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
```

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

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### 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 = '-')
```