The ionio-illustrate package

Version 0.1.1

1. Introduction

This package implements a Cetz chart-like object for displaying mass spectrometric data in Typst documents. It allows for individually styled mass peaks, callouts, titles, and mass callipers.

2. Usage

This is the minimal starting point:

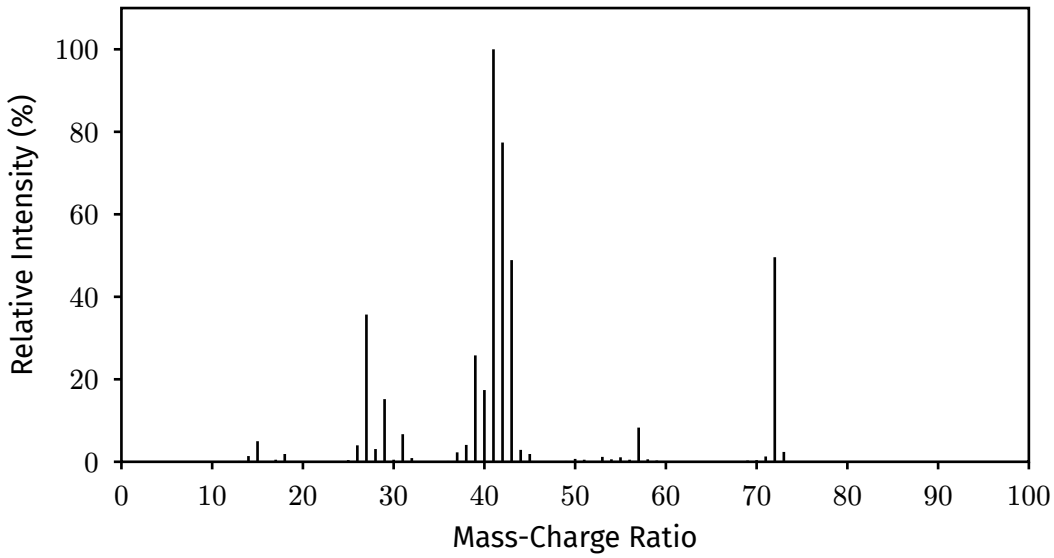
Example

```
#import "@preview/ionio-illustrate:0.1.1": *
#let data = csv("isobutelene_epoxide.csv")

#let ms = mass-spectrum(massspec, args: (
  size: (12,6),
  range: (0,100),
))

#figure((ms.display)())
```

The above code produces the following content:



It is important to note at this point that the syntax for interacting with mass spectrum objects will certainly change with the introduction of a native type system. This document will be updated to reflect this upon implementation of those changes.

2.1. mass-spectrum()

The mass-spectrum() function takes two positional arguments:

- data (array or dictionary): This is a 2-dimensional array relating mass-charge ratios to their intensities. By default, the first column is the mass-charge ratio and the second column is the intensity.
- args (dictionary): This contains suplemental data that can be used to change the style of the mass spectrum, or to add additional content using provided functions (see Section 2.1.7).

The defaults for the args dictionary are shown below:

```
keys: (
  mz: 0,
  intensity: 1
),
size: (auto, 1),
range: (40, 400),
style: mass-spectrum-default-style,
labels: (
  x: [Mass-Charge Ratio],
  y: [Relative Intensity (%)]
),
linestyle: (this, idx)=>{},
plot-extras: (this)=>{},
```

2.1.1. keys

The keys entry in the args positional argument is a dictionary that can be used to change which fields in the provided data array / dictionary are to be used to plot the mass spectrum. An example usage of this may be to store several mass spectra within a single datafile.

Info

Note that arrays are 0-index based.

Example

```
#let ms = mass-spectrum(massspec, args: (
  keys: (
    mz: 0, // mass-charge is contained in the first column
    intensity: 1 // intensity is contained in the second column
  )
))
```

2.1.2. size

The keys entry in the args positional argument is a tuple specifying the size of the mass spectrum on the page, in Cetz units.

Example

```
#let ms = mass-spectrum(massspec, args: (
  size: (12,6)
))
```

2.1.3. range

The range entry in the args positional argument is a tuple specifying the min and the max of the mass-charge axis.

```
#let ms = mass-spectrum(massspec, args: (
  range: (0,100) // Show mass spectrum between 0 m/z and 100 m/z
))
```

2.1.4. style

The style entry in the args positional argument is a cetz style dictionary. It is presently unused until it is better understood where styling is appropriate.

2.1.5. labels

The labels entry in the args positional argument is a dictionary specifying the labels to be used on each axis.

Note that if you provide this entry, you must provide both child entries.

```
#let ms = mass-spectrum(massspec, args: (
  labels: (
    x: [Mass-Charge Ratio],
    y: [Relative Intensity \[%\]]
  )
))
```

2.1.6. linestyle

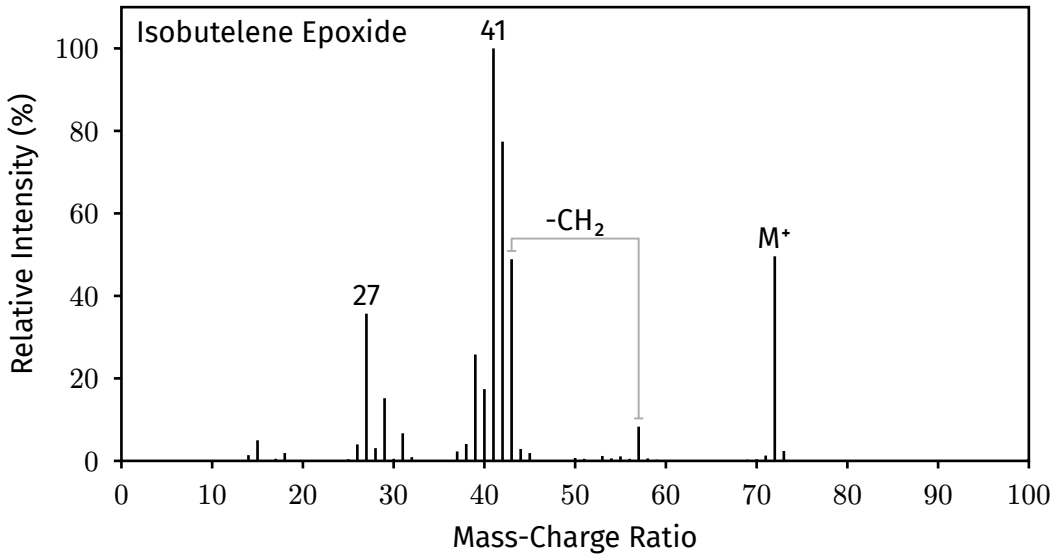
The linestyle entry in the args positional argument is a function taking two parameters: this (refering to the #ms object), and idx which represents the mass-charge ratio of the peak being drawn. Returning a cetz style dictionary will change the appearence of the peaks. This may be used to draw the reader's attention to a particular mass spectrum peak by colouring it in red, for example.

```
#let ms = mass-spectrum(massspec, args: (
  linestyle: (this, idx)=>{
      if idx==41 {return (stroke: red)}
    }
))
```

2.1.7. plot-extras

The plot-extras entry in the args positional argument is a function taking one parameter, this, which refers to the #ms object. It can be used to add additional content to a mass spectrum using provided functions

```
#let ms = mass-spectrum(massspec, args: (
  size: (12,6), range: (0,100),
  plot-extras: (this) => {
    (this.callout-above)( 72, content: MolecularIon())
    (this.callout-above)(27)
    (this.callout-above)( 41)
    (this.callipers)( 43, 57, content: [\-CH#sub("2")])
    (this.title)([Isobutelene Epoxide])
  }
))
#figure((ms.display)())
```



2.2. Method functions

This section briefly outlines method functions and where/why they might be used

2.2.1. `#ms.display()`

the `#ms.display` method is used to place a mass spectrum within a document. It can be called several times. It **must not** be called within the context of a `plot-extras(this)` function.

2.2.2. `#ms.title(content)`

the `#ms.title` method allows the addition of a title to a mass spectrum. It should be called within the context of a `plot-extras(this)` function.

2.2.3. `#ms.callout-above(mz, content: [])`

the `#ms.callout-above` method places a callout slightly above the intensity peak for a given mass-charge ratio. It should be called within the context of a `plot-extras(this)` function.

2.2.4. `#ms.callipers(mz1, mz2, content: none, height: none)`

the `#ms.callipers` method places a mass callipers between two mass spectrum peaks, along with any desired content centered above the callipers. If `height` is not specified, it is set automatically to a few units above the most intense peak. If `content` is not specified, it is set automatically to represent the loss of mass between the specified peaks. It should be called within the context of a `plot-extras(this)` function.