Reference

Retention time alignment

The alignment of retention times between MS runs done with MassChroQ3 are represented as follow in the JSON output

MS run alignment data

```
{
    "corrections": {
        "msruna1": {
            "aligned": [],
            "ms2_delta_rt": {
                "x": [],
                "y": []
            },
            "ms2_mean": [],
            "ms2_median": [],
            "original": []
        },
        "msruna2": {
            "aligned": [],
            "ms2_delta_rt": {
                "x": [],
                "y": []
            },
            "ms2_mean": [],
            "ms2_median": [],
            "original": []
        },
        "msruna3": {
            "aligned": [],
            "ms2_delta_rt": {
                "x": [],
                "y": []
            },
            "ms2_mean": [],
            "ms2_median": [],
            "original": []
        },
    },
    "msrun_ref": "msruna4"
}
```
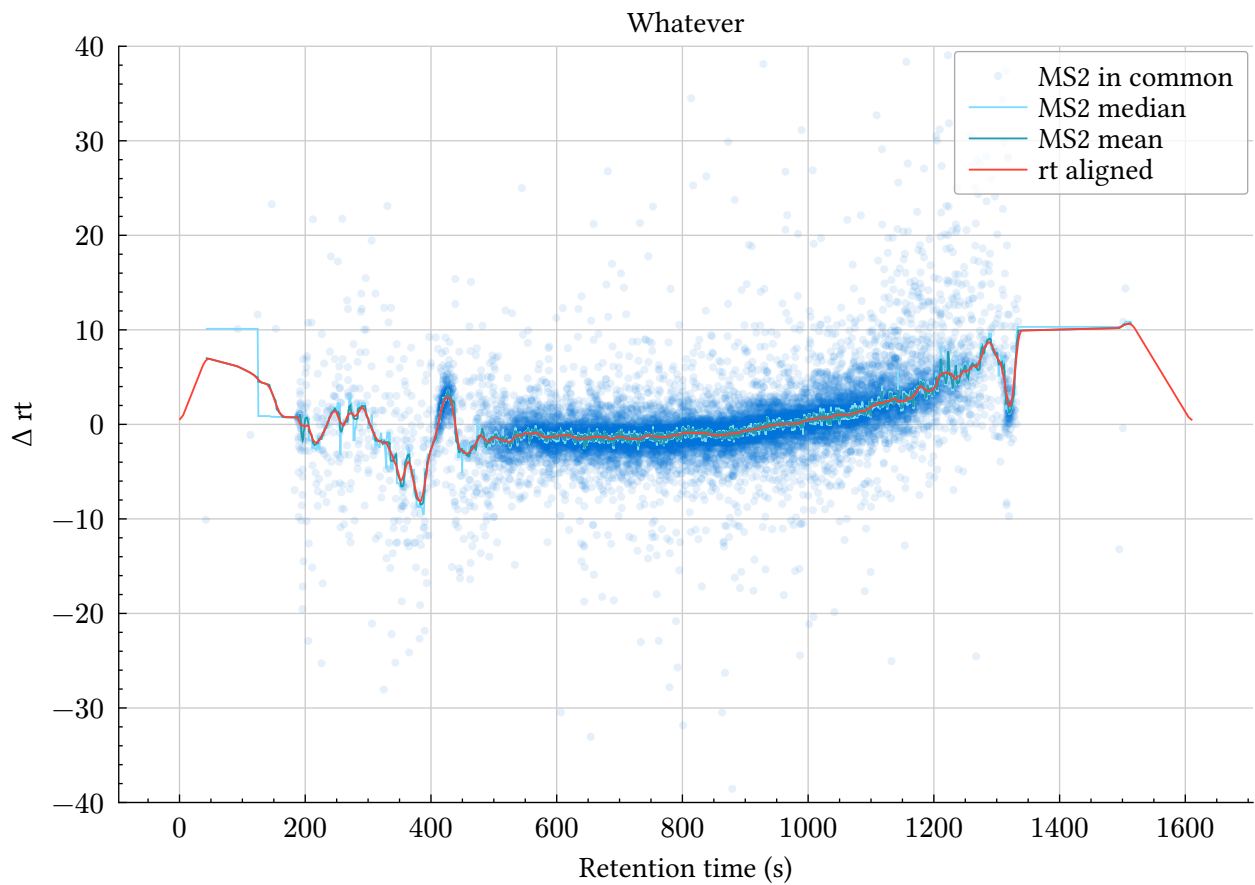
Example :

```
#import "@local/proteograph:0.1.0": *

#let rt_align = json("../examples/data/one_alignment.json")
#rtalign-plot(title: "Whatever", ylim: (-40,40),
  ms2-delta-rt: rt_align.ms2_delta_rt,
  aligned: rt_align.aligned,
  ms2-mean: rt_align.ms2_mean,
```

```
ms2-median: rt_align.ms2_median,
original: rt_align.original)
```

Result :

Retention time alignment full documentation

- rtalign-plot()

rtalign-plot

retention time delta plot between MS runs plot.

Parameters

```
rtalign-plot(
  width: length relative ,
  height: length relative ,
  xlim: auto array ,
  ylim: auto array ,
  title,
  original,
  aligned,
  ms2-delta-rt,
  ms2-mean,
  ms2-median
) -> content
```

width   `length` or `relative`

The width of the diagram. This can be
- A `length`; in this case, it defines just the width of the data area, excluding axes, labels, title etc.
- A `ratio` or `relative` where the ratio part is relative to the width of the parent that the diagram is placed in. This is not allowed if the parent has an unbounded width, e.g., a page with `width: auto`.

Default: `15cm`

height   `length` or `relative`

The height of the diagram. This can be
- A `length`; in this case, it defines just the height of the data area, excluding axes, labels, title etc.
- A `ratio` or `relative` where the ratio part is relative to the height of the parent that the diagram is placed in. This is not allowed if the parent has an unbounded height, e.g., a page with `height: auto`.

Default: `10cm`

xlim   `auto` or `array`

Data limits along the x-axis (retention time in seconds). Expects auto or a tuple (min, max) where min and max may individually be auto

Default: `auto`

ylim   `auto` or `array`

Data limits along the y-axis (retention time delta in seconds). Expects auto or a tuple (min, max) where min and max may individually be auto

Default: `(-40,40)`

MS2 spectra

Simple MS2 spectra
The spectra is a dictionnary containing 2 arrays of floats : mz and intensity

spectra dictionnary
```
{
        "intensity": [
            2,
            2,
            100,
            5,
            7,
            2
        ],
```

```
    "mz": [
        155.081,
        157.097,
        157.133,
        158.092,
        158.137,
        159.076
    ]
}
```
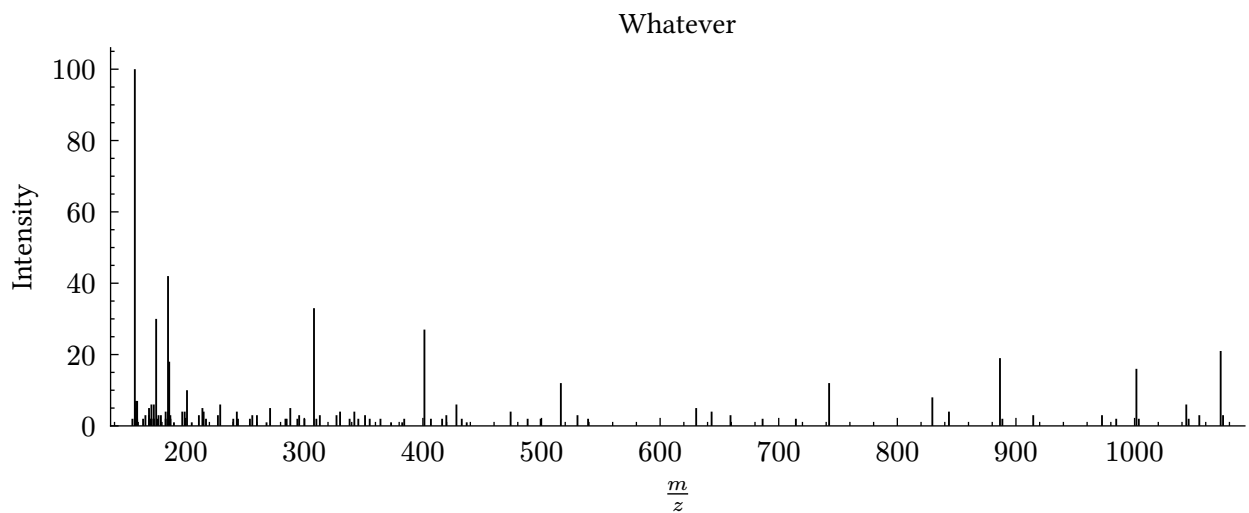
Example :

```
#import "@local/proteograph:0.1.0": *

#let complete_psm = json("../examples/data/complete_psm.json")
#ms2spectra-plot(height: 5cm, title: "Whatever", spectra: complete_psm.spectra)
```

Result :

MS2 spectra with ion annotations

This example shows an MS2 spectra with ion series annotation

The ion annotations are described in a dictionnary :

ion-series dictionnary

```
{
        "a": [
            {
                "charge": 1,
                "intensity": 100,
                "mz": 157.133,
                "mzth": 157.13353961189497,
                "size": 2
            }
        ],
        "b": [
            {
                "charge": 1,
```

```
            "intensity": 42,
            "mz": 185.128,
            "mzth": 185.12845423145498,
            "size": 2
        },
        {
            "charge": 1,
            "intensity": 3,
            "mz": 256.165,
            "mzth": 256.16556801702,
            "size": 3
        }
    ]
}
```

The first key is the ion series name as follow :

y, b, yp, ystar, y*, yO, x, bstar, b*, bO, a, astar, aO, c, z, bp

and any ion can be described by :

- ion-description()

ion-description
Ion description

Parameters

```
ion-description(
    "charge": integer ,
    "intensity": float ,
    "mz": float ,
    "mzth": float ,
    "size": integer
)
```

"charge" `integer`

Ion charge

Default: 1

"intensity" `float`

Ion intensity

Default: none

"mz" `float`

Ion experimental mass on charge ratio

Default: none

"mzth" `float`

Ion theoretical mass on charge ratio. **Optional**.

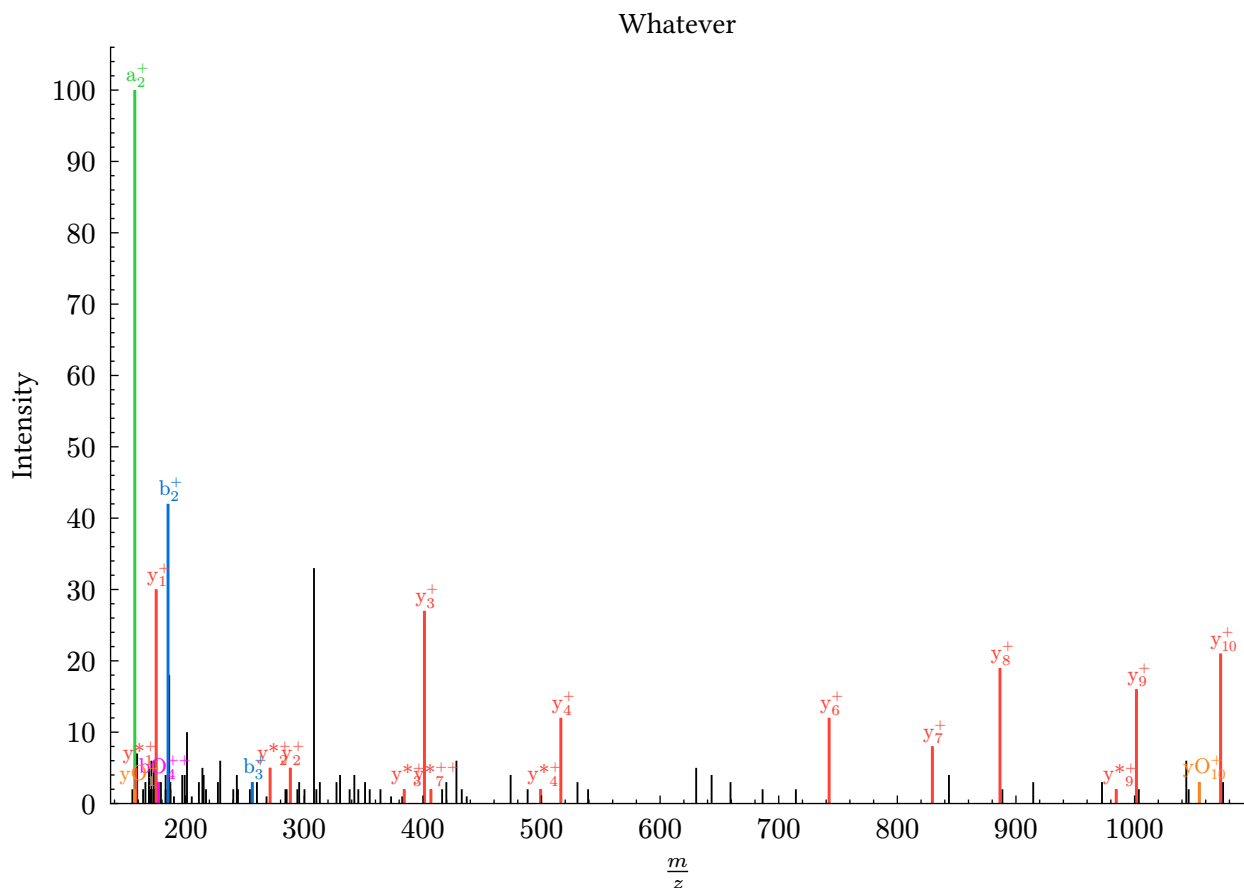Default: none

"size" `integer`

Ion size : number of residues for this fragment

Default: 1

Example :

```
#import "@local/proteograph:0.1.0": *

#let complete_psm = json("../examples/data/complete_psm.json")
#ms2spectra-plot(title: "Whatever", spectra: complete_psm.spectra, ion-series:
complete_psm.ion-series)
```

Result :
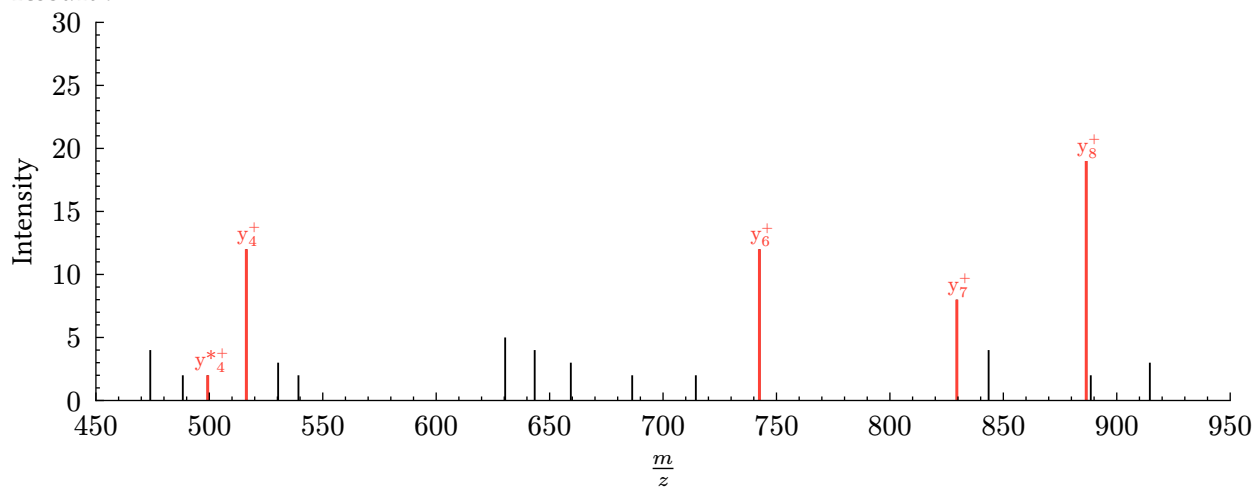

MS2 spectra zoom (mz_range and intensity)

This example shows an MS2 spectra zoomed on a specific m/z range and maximum intensity.

Example :

```
#import "@local/proteograph:0.1.0": *

#let complete_psm = json("../examples/data/complete_psm.json")
```

```
#ms2spectra-plot(width: 15cm, height: 5cm, spectra: complete_psm.spectra, ion-series:
complete_psm.ion-series, mz-range: (450, 950), max-intensity: 30)
```

Result :

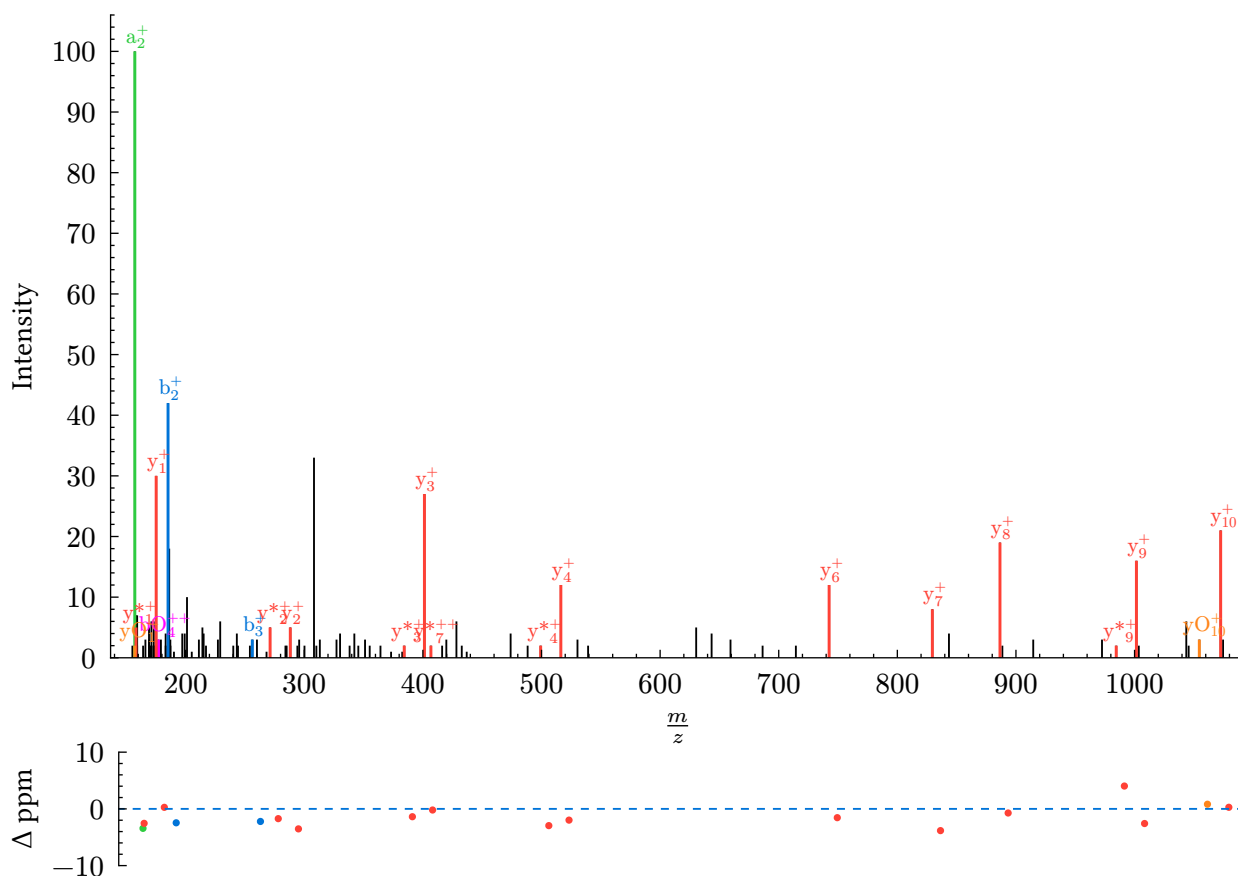**MS2 spectra with ion annotations and MS2 fragments mass delta**

This example shows an MS2 spectra with ion series annotation

Example :

```
#import "@local/proteograph:0.1.0": *

#let complete_psm = json("../examples/data/complete_psm.json")
#ms2spectra-plot(width: 15cm, height: 10cm, spectra: complete_psm.spectra, ion-
series: complete_psm.ion-series, delta-fragments: true)
```

Result :

MS2 spectra full documentation

- ms2spectra-plot()

ms2spectra-plot

Generates an annotated MS2 spectra plot.

Parameters

```
ms2spectra-plot(
    width: length relative ,
    height: length relative ,
    title: str content ,
    mz-range: none array ,
    max-intensity: none float ,
    spectra: none dictionary ,
    ion-series,
    delta,
    delta-fragments: bool
) -> content
```

width `length` or `relative`

The width of the diagram. This can be
- A `length`; in this case, it defines just the width of the data area, excluding axes, labels, title etc.
- A `ratio` or `relative` where the ratio part is relative to the width of the parent that the diagram is placed in. This is not allowed if the parent has an unbounded width, e.g., a page with `width: auto`.

Default: `15cm`

height `length` or `relative`

The height of the diagram. This can be
- A `length`; in this case, it defines just the height of the data area, excluding axes, labels, title etc.
- A `ratio` or `relative` where the ratio part is relative to the height of the parent that the diagram is placed in. This is not allowed if the parent has an unbounded height, e.g., a page with `height: auto`.

Default: `10cm`

title `str` or `content`

Shows the plot title. **Optional**.

Default: `none`

mz-range `none` or `array`

m/z range to display. **Optional**.

Example: (`450`, `950`)

Default: `none`

max-intensity `none` or `float`

maximum intensity to display. **Optional**.

Example: `30000`

Default: `none`

spectra `none` or `dictionary`

Mass spectra values. **Optional**. a dictionary with the keys `mz` (array of mass to charge ratios) and `intensity` (array of intensities) with the same length for each array

(e.g., `spectra: (mz: (256.45, 356.89, 523.78), intensity: (200, 298 ,253)))`)

```
#import "@local/proteograph:0.1.0": *
#set text(size: 12pt)
#ms2spectra-plot( spectra: (mz: (256.45,
356.89, 523.78), intensity: (200, 298,
253)))
```
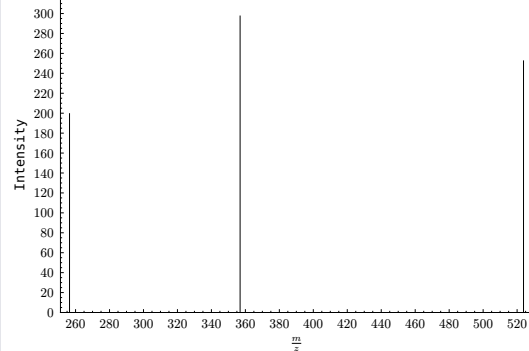

Default: `none`

---

delta-fragments `bool`

Whether to clip the matched ion masss delta to the plot. **Optional**.

Default: `false`