

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"
  }
}
```

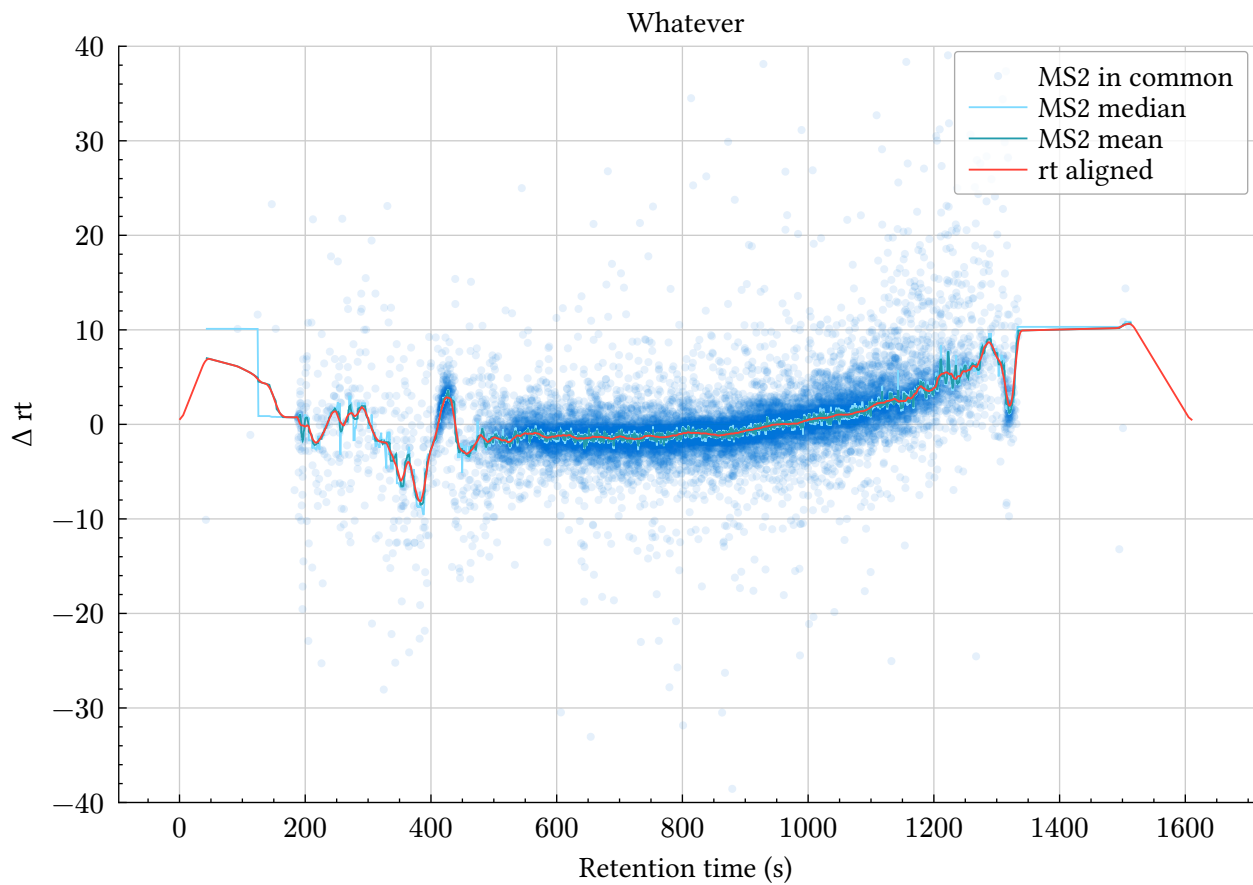
Example :

```
#import "@local/teproteograph: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 dictionary containing 2 arrays of floats : `mz` and `intensity`

spectra dictionary

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

```

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

```

Example :

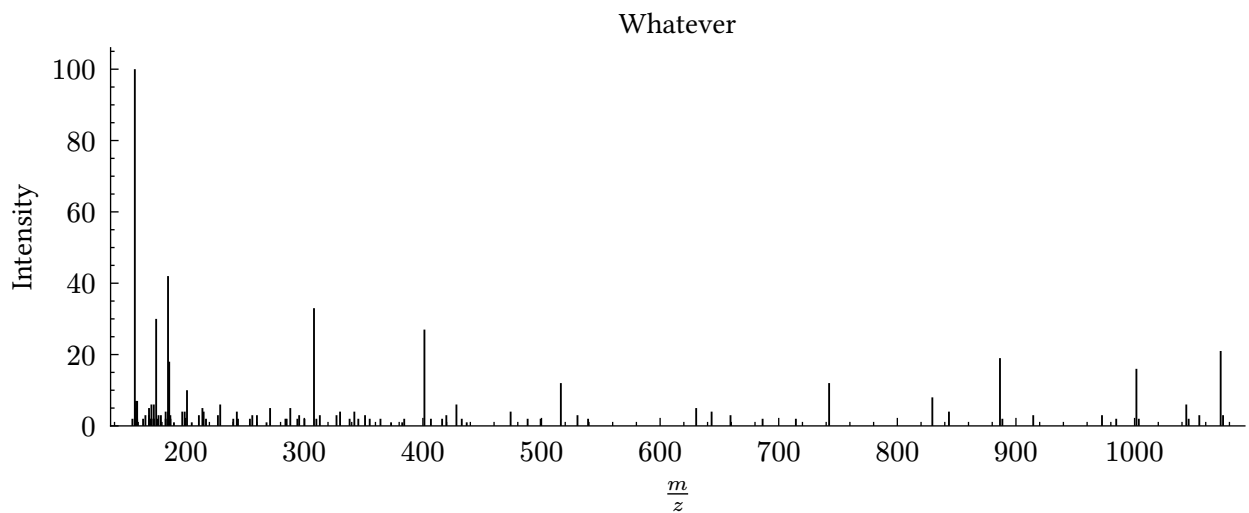
```

#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 dictionary :

ion-series dictionary

```

{
  "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

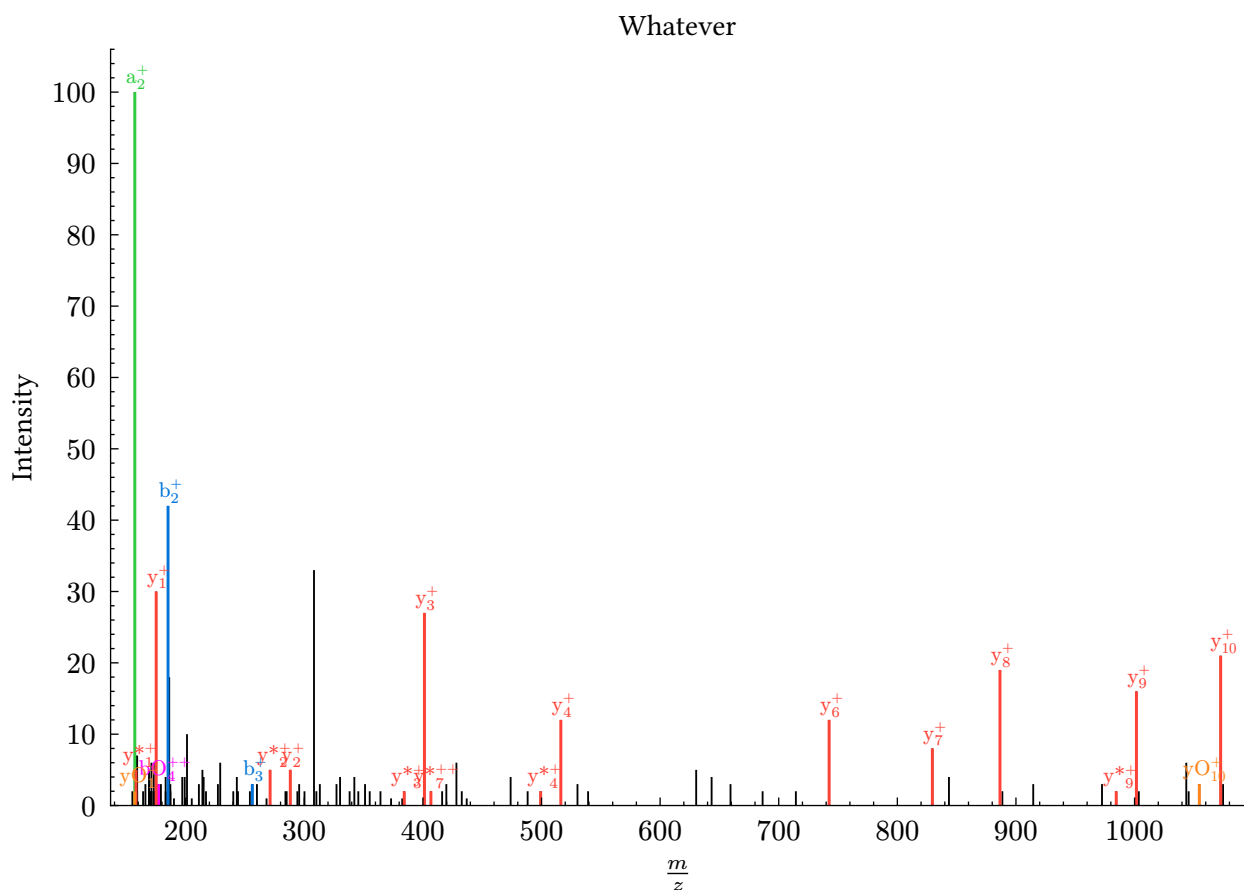
Ion size : number of residues for this fragment

Default: 1

Example :

```
#import "@local/teproteograph: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)

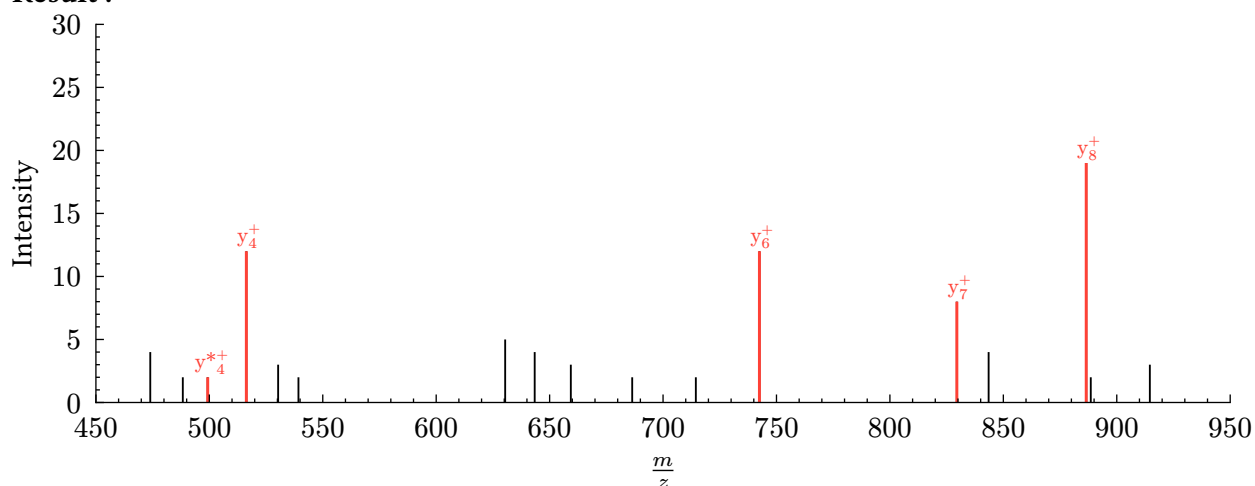
This example shows an MS2 spectra zoomed on a specific m/z range and maximum intensity.

Example :

```
#import "@local/teproteograph: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

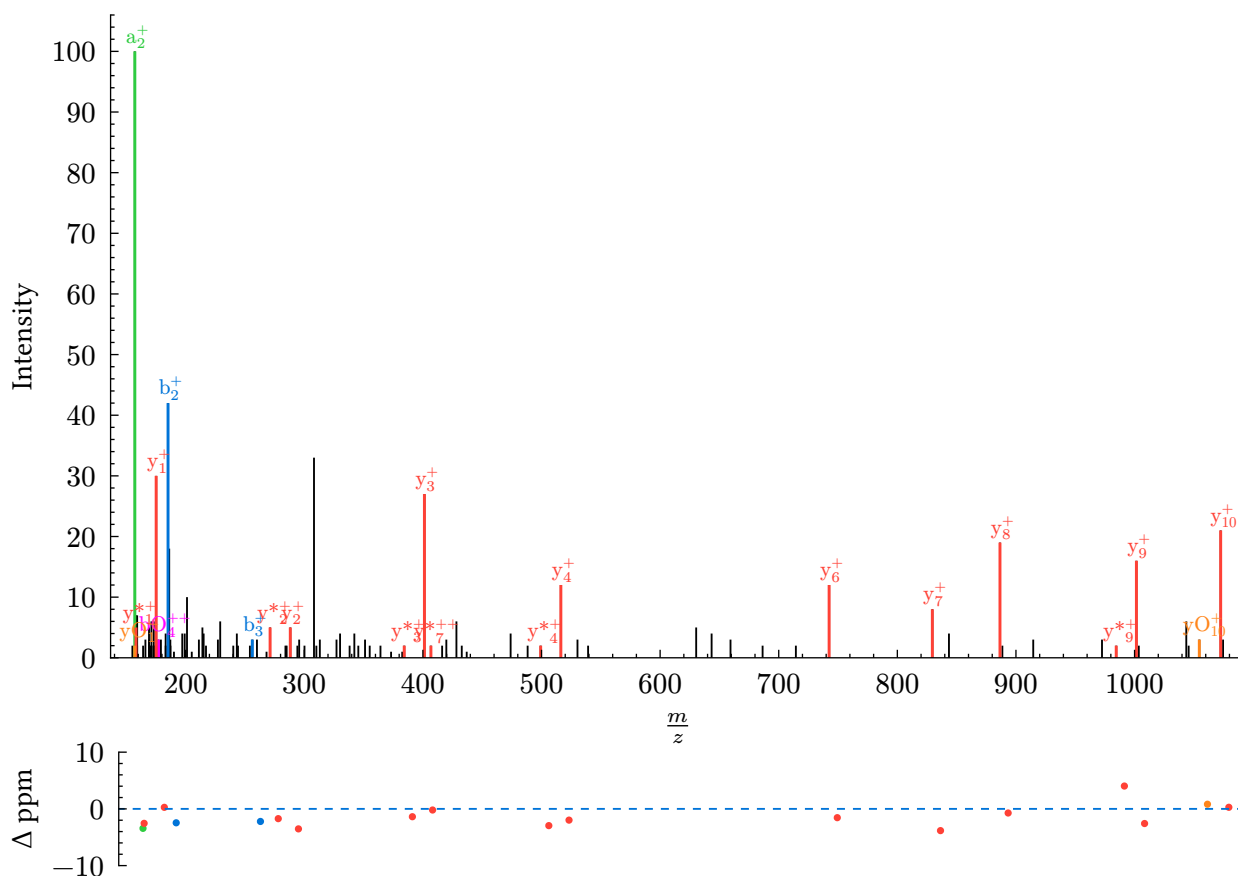
This example shows an MS2 spectra with ion series annotation

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`

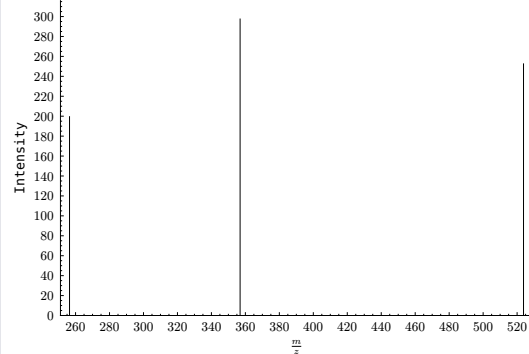
Default: `none`

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/tegraph: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 mass delta to the plot. **Optional.**

Default: `false`