

# Proteograph

Typst proteomics package

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<https://codeberg.org/olangella/proteograph>

Olivier Langella

## ABSTRACT

**proteograph** is a package defining `Typst` functions dedicated to proteomics.

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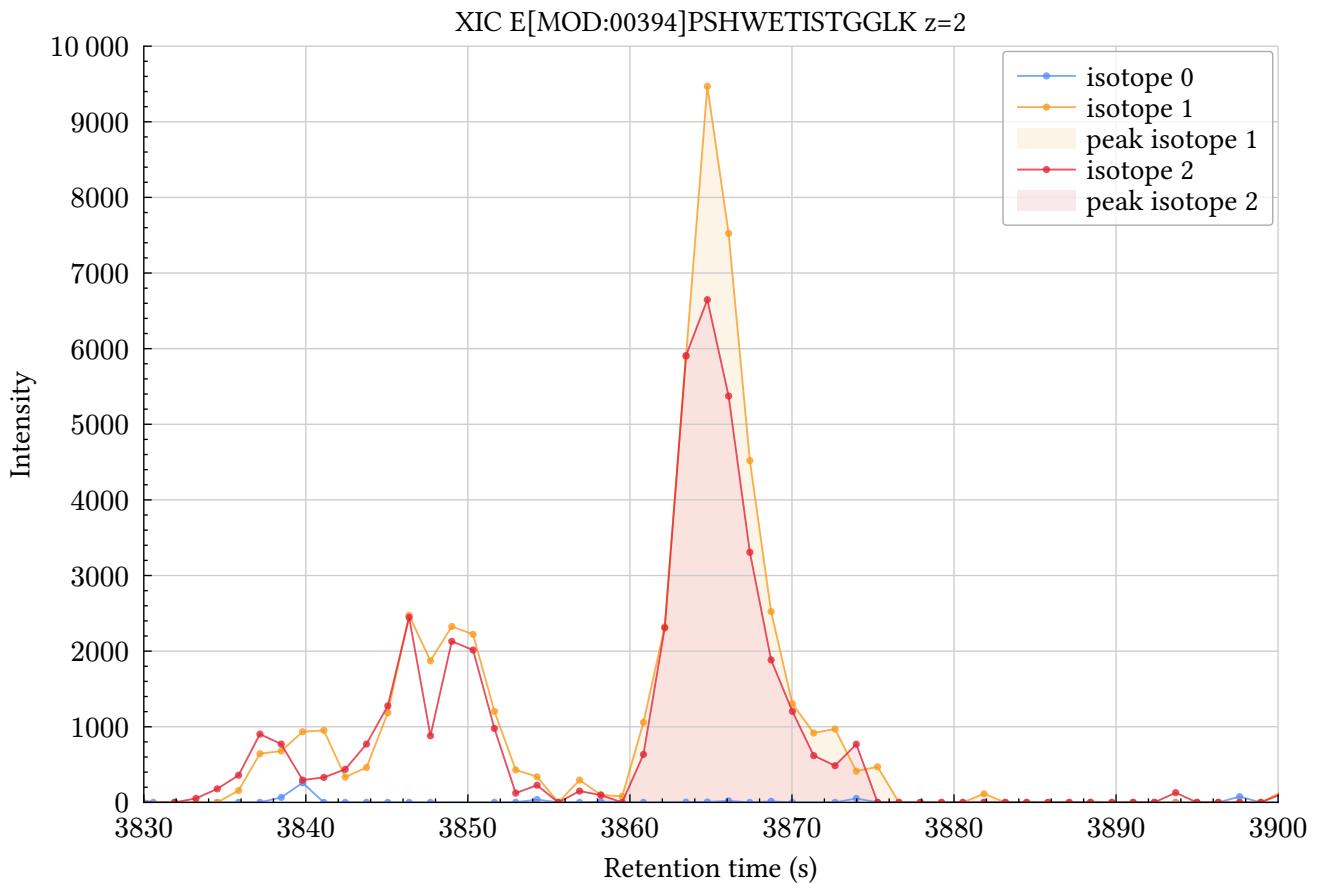
## REFERENCE

### XIC (eXtracted Ion Chromatogram) plot

**Example :**

```
#import "@preview/proteograph:0.2.1": *  
  
#let data_json = json("../examples/data/pepa1b35.json")  
  
#let xic0 = data_json.found_list_first_pass.first().xics.first().trace  
#xic0.insert("title","isotope 0")  
#let xic1 = data_json.found_list_first_pass.first().xics.at(1).trace  
#xic1.insert("title","isotope 1")  
#xic1.insert("peak-  
begin",data_json.found_list_first_pass.first().xics.at(1).peak.rt.first())  
#xic1.insert("peak-  
end",data_json.found_list_first_pass.first().xics.at(1).peak.rt.last())  
#let xic2 = data_json.found_list_first_pass.first().xics.at(2).trace  
#xic2.insert("title","isotope 2")  
#xic2.insert("peak-  
begin",data_json.found_list_first_pass.first().xics.at(2).peak.rt.first())  
#xic2.insert("peak-  
end",data_json.found_list_first_pass.first().xics.at(2).peak.rt.last())  
  
#xic-plot(height: 10cm, title: "XIC E[MOD:00394]PSHWETISTGGLK z=2", rt-range: (3830,  
3900), max-intensity: 10000, xic0,xic1, xic2)
```

## Result :



## XIC plot full documentation

- [xic-isotope-plot\(\)](#)
- [xic-plot\(\)](#)

### xic-isotope-plot

Generates a XIC plot separating istope pattern by charge

#### Parameters

```
xic-isotope-plot(  
    width: length relative,  
    height: length relative,  
    rt-range: auto array,  
    max-intensity: none float,  
    title: content,  
    ..xic-item: dictionary  
) -> 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`

**rt-range** `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`

**max-intensity** `none` or `float`

Maximum intensity to display. **Optional**.

Example: `30000`

Default: `none`

**title** `content`

Graph title

Default: `none`

## **.xic-item** dictionary

dictionary containing XIC data

```

1  /// XIC dictionary structure
2  #let xic_item = (
3    /// Array of retention times values
4    "x": (),
5    /// Array of intensity values
6    "y": (),
7    /// Title for this XIC
8    "title": "title for this XIC"
9    /// Detected peak retention time start. *Optional*.
10   "peak-begin": 3500,
11   /// Detected peak retention time end. *Optional*.
12   "peak-end": 3500,
13   /// Charge.
14   "charge": none,
15   /// Isotope number.
16   "isotope": none,
17 )

```

typc

## **xic-plot**

Generates a XIC plot.

### Parameters

```

xic-plot(
  width: length relative ,
  height: length relative ,
  rt-range: auto array ,
  max-intensity: none float ,
  title: content ,
  ..xic-item: dictionary
) -> 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`

**rt-range** `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`

**max-intensity** `none` or `float`

Maximum intensity to display. **Optional**.

Example: `30000`

Default: `none`

**title** `content`

Graph title

Default: `none`

**.xic-item** `dictionary`

dictionary containing XIC data

```
1  /// XIC dictionary structure
2  #let xic_item = (
3    /// Array of retention times values
4    "x": (),
5    /// Array of intensity values
6    "y": (),
7    /// Title for this XIC
8    "title": "title for this XIC"
9    /// Detected peak retention time start. *Optional*.
10   "peak-begin": 3500,
11   /// Detected peak retention time end. *Optional*.
12   "peak-end": 3500,
13 )
```

typc

## 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*

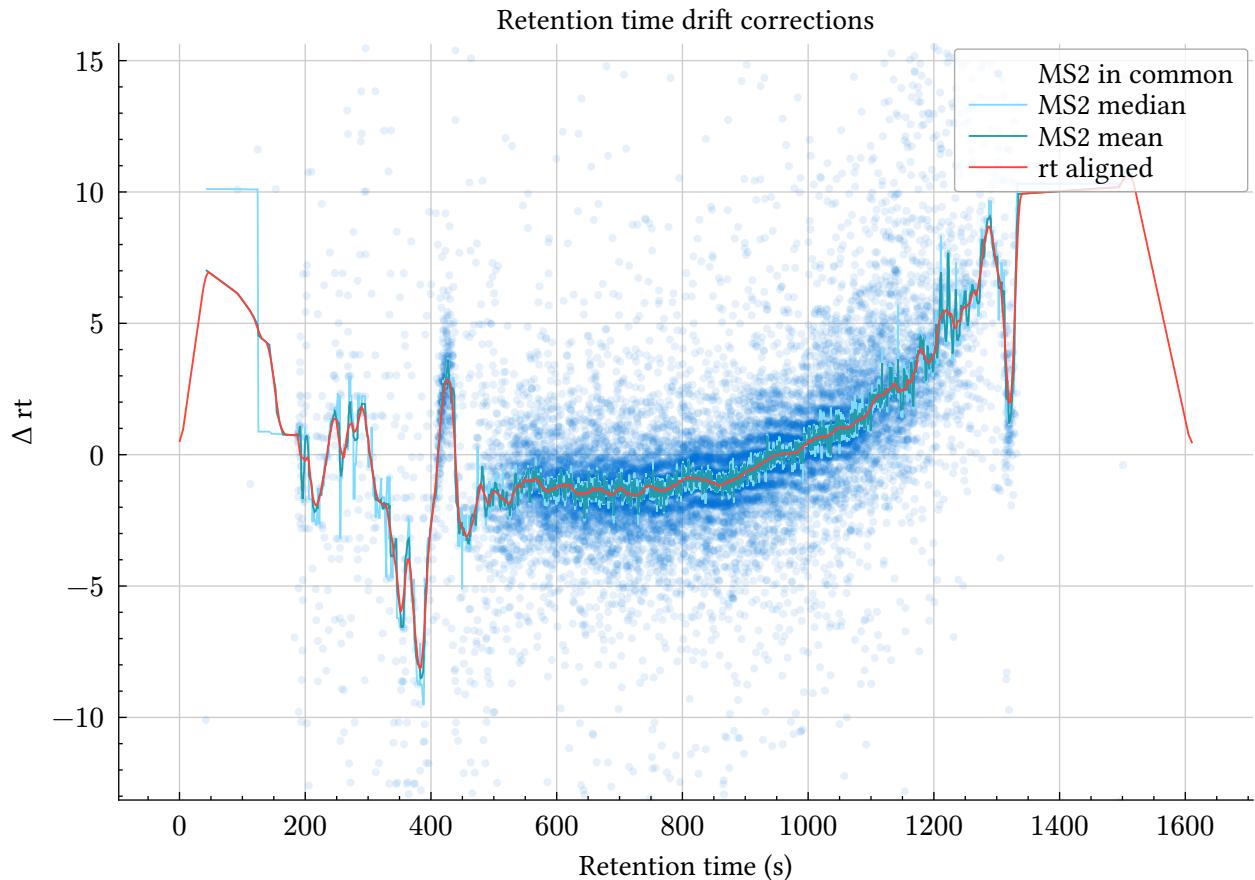
```
{  
    "corrections": {  
        "msruna1": {  
            "aligned": [],  
            "ms2_delta_rt": {  
                "x": [],  
                "y": []  
            },  
            "ms2_mean": [],  
            "ms2_median": [],  
            "original": []  
        },  
        "msruna2": {  
            "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 "@preview/proteograph:0.2.1": *  
  
#let rt_align = json("../examples/data/one_alignment.json")  
#rtalign-plot(title: "Retention time drift corrections", ylim: auto,  
    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: `auto`

## MS2 spectra

### Simple MS2 spectra

The spectra is a dictionary containing 2 arrays of floats : mz and intensity

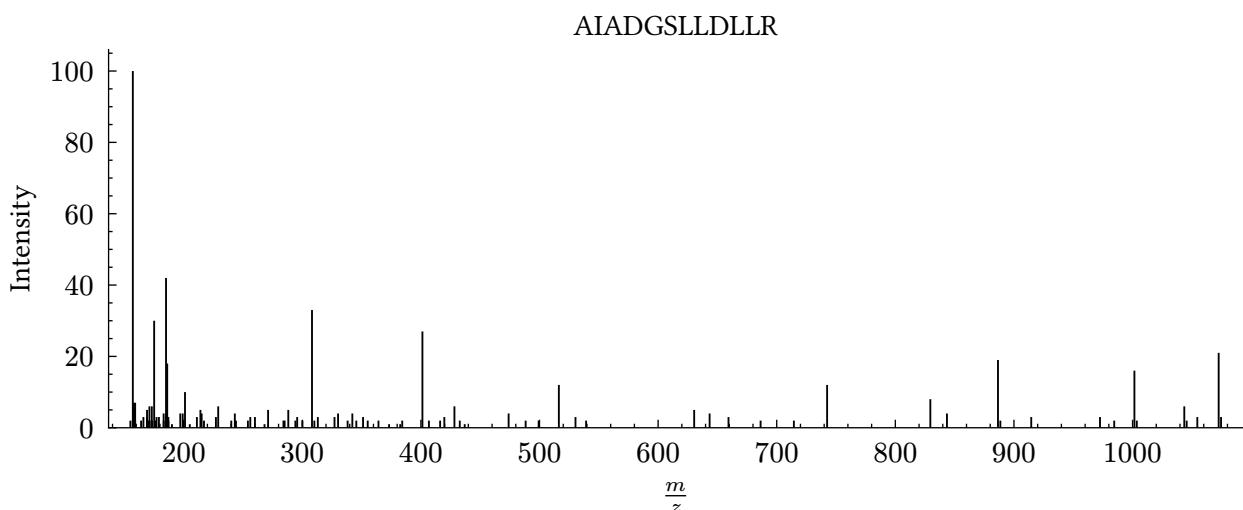
```
spectra dictinonary
{
    "intensity": [
        2,
        2,
        100,
        5,
        7,
        2
    ],
    "mz": [
        155.081,
        157.097,
        157.133,
        158.092,
        158.137,
        159.076
    ]
}
```

### Example :

```
#import "@preview/proteograph:0.2.1": *

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

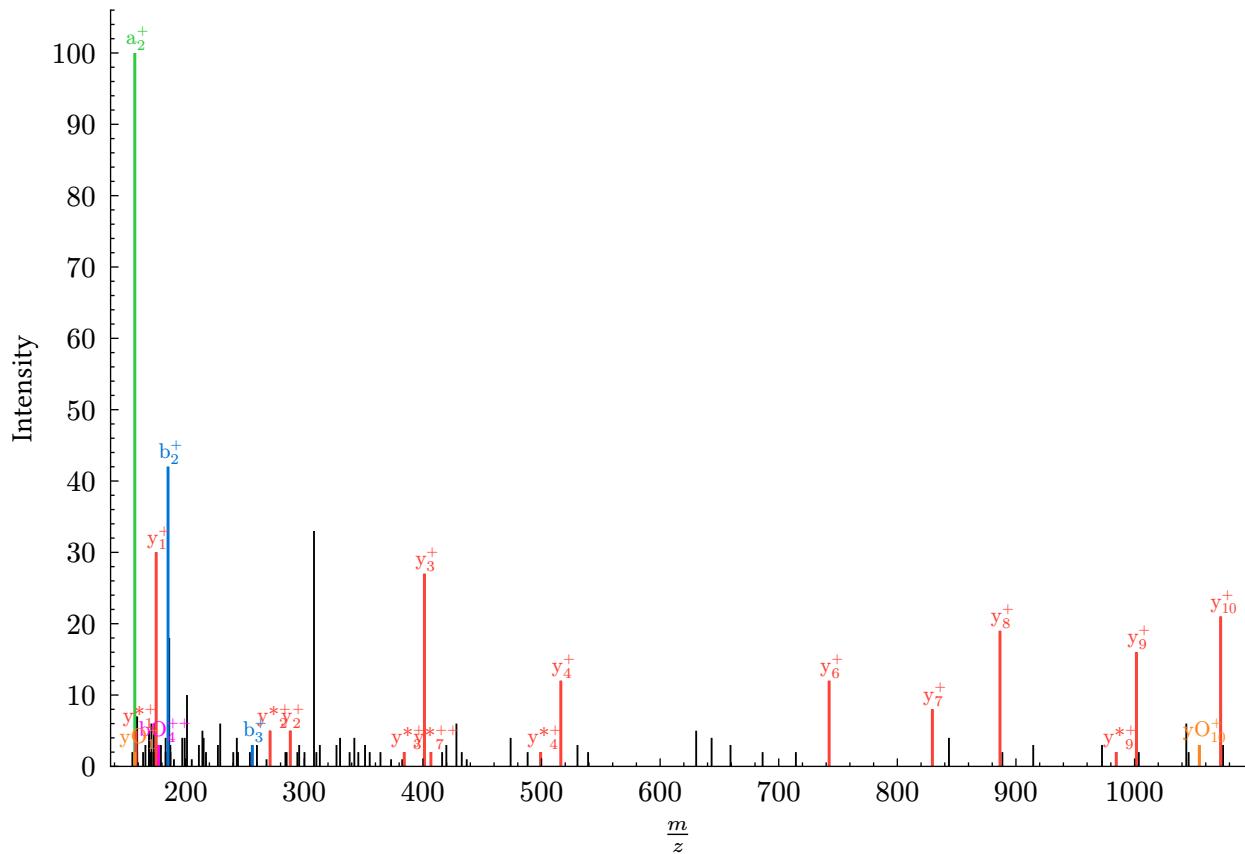
Default: `1`

## Example :

```
#import "@preview/proteograph:0.2.1": *  
  
#let complete_psm = json("../examples/data/complete_psm.json")  
#ms2spectra-plot(title: "AIADGSLLDLLR", spectra: complete_psm.spectra, ion-series:  
complete_psm.ion-series)
```

## **Result :**

AIADGSLLDLLR



## MS2 spectra zoom (mz\_range and intensity)

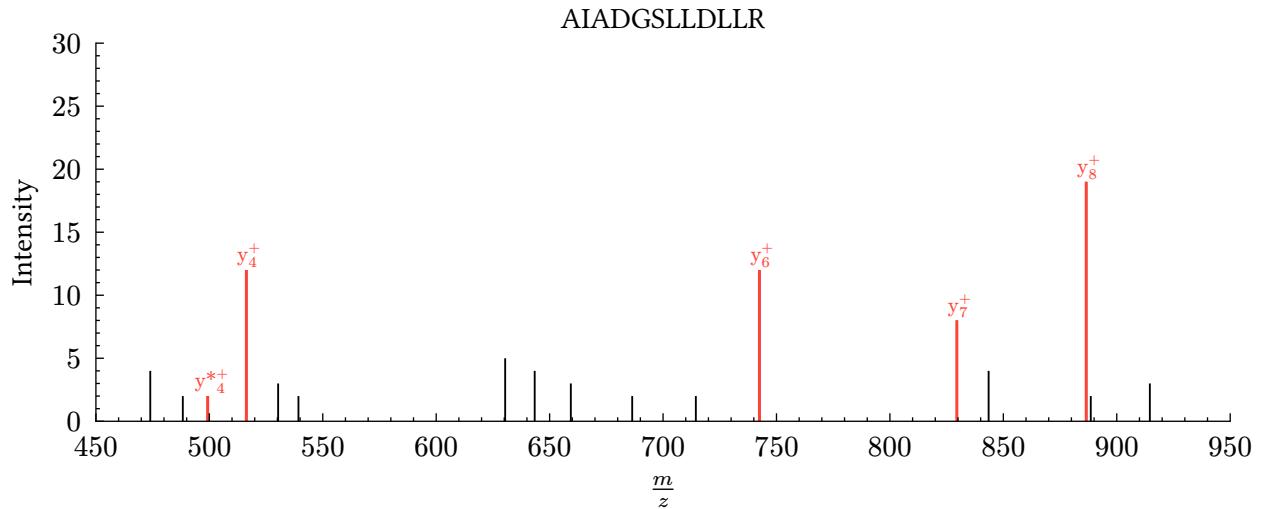
This example shows an MS2 spectra zoomed on a specific m/z range and maximum intensity.

## Example :

```
#import "@preview/proteograph:0.2.1": *
```

```
#let complete_psm = json("../examples/data/complete_psm.json")
#ms2spectra-plot(width: 15cm, height: 5cm, title: "AIADGSLLDLLR", spectra:
complete_psm.spectra, ion-series: complete_psm.ion-series, mz-range: (450, 950), max-
intensity: 30)
```

## Result :



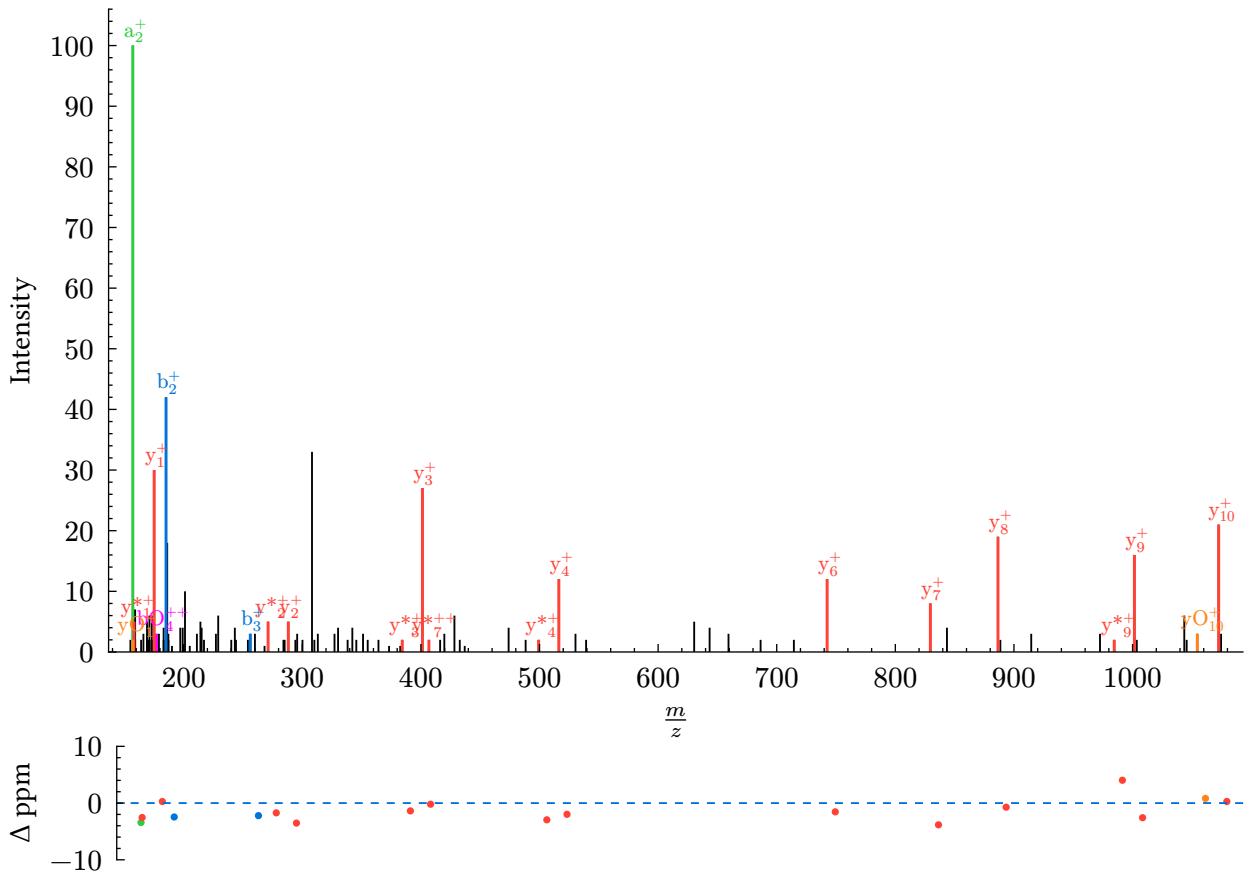
## MS2 spectra with ion annotations and MS2 fragments mass delta

This example shows an MS2 spectra with ion series annotation

### Example :

```
#import "@preview/proteograph:0.2.1": *  
  
#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 with ion annotations and highlighted mass delta between peaks

The space between two peaks can be highlighted and manually annotated using an array defined as follow

*Highlight space between peaks array*

```
[  
{  
  "ion": "y",  
  "mz": [401.287,516.313],  
  "level": 1,  
  "label": "D"  
},  
{  
  "ion": "y",  
  "mz": [742.481,829.511],  
  "level": 1,  

```

```

    "ion": "y",
    "mz": [886.535,1001.56],
    "level": 1,
    "label": "D"
}
]

```

### Example :

```

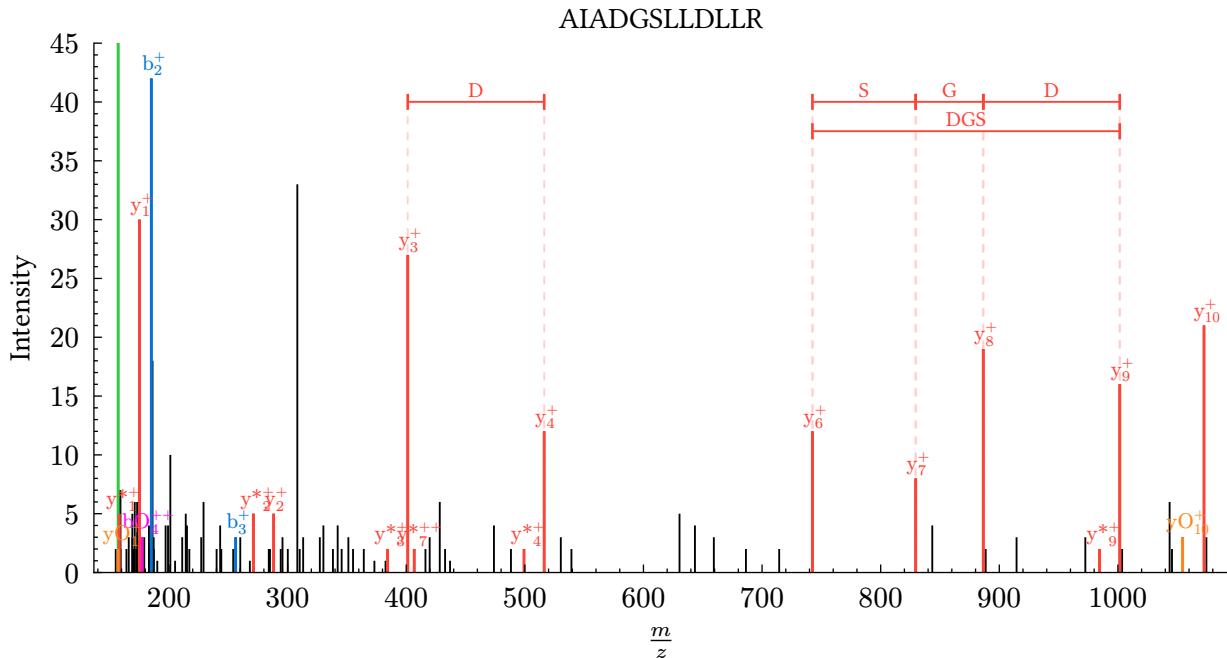
#import "@preview/proteograph:0.2.1": *

#let delta_arr = (
(
    "ion": "y",
    "mz": (401.287,516.313),
    "level": 1,
    "label": "D"
),
(
    "ion": "y",
    "mz": (742.481,829.511),
    "level": 1,
    "label": "S"
),
(
    "ion": "y",
    "mz": (829.511,886.535),
    "level": 1,
    "label": "G"
),
(
    "ion": "y",
    "mz": (886.535,1001.56),
    "level": 1,
    "label": "D"
),
(
    "ion": "y",
    "mz": (742.481,1001.56),
    "level": 2,
    "label": "DGS"
)
)

#let complete_psm = json("../examples/data/complete_psm.json")
#ms2spectra-plot(width: 15cm, height: 7cm, max-intensity: 45, title: "AIADGSLLDLLR",
spectra: complete_psm.spectra, ion-series: complete_psm.ion-series, delta: delta_arr)

```

## 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`

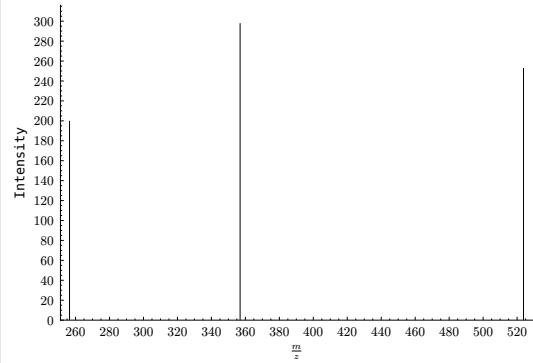
**spectra** none or dictionary

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))`)

```
1 #import "@preview/  
proteograph:0.2.1": *  
2 #set text(size: 12pt)  
#ms2spectra-plot( spectra: (mz:  
3 (256.45, 356.89, 523.78), intensity:  
(200, 298, 253)))
```



Default: `none`

**delta-fragments** bool

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

Default: `false`

## Protein sequence

### Example :

```
#import "@preview/proteograph:0.2.1": *
```

```
#protein-sequence(line-length: 60,
```

```
"MASTKAPGPGEKHSIDAQLRQLVPGKVSEDDKLIEYDALLVDRFLNILQDLHGPSLREFVQE
```

### Result :

```
0 MASTKAPGPGEKHSIDAQLRQLVPGKVSEDDKLIEYDALLVDRFLNILQDLHGPSLREF
60 VQECEVSADYEKGDTTKLGELGAKLTGLAPADAILVASSILHMLNLANLAEEVQIAHR
120 RRNSKLKKGGFADEGSATTESDIEETLKRLVSEVGKSPEEVFEALKNQTVDLVFTAHPHQ
180 SARRSLLQKNARIRNCLTQLNAKDITDDDQKELDEALQREIQAAFRTDEIRRAQPTPQDE
240 MRYGMSYIHETVWKGVPKFLRRVTALKNIGINERLPYNVSLIRFSSWMGGDRDGPNPRVT
300 PEVTRDVCLLARMMAANLYIDQIELMFELSMWRCNDELRVRAEELHSSSGSKVTKYYIE
360 FWKQIPPNEPYRVLGHVRDKLYNTRERARHLLASGVSEISAESSFTSIEEFLEPLELCY
420 KSLCDCGDKAIADGSLLDLLRQVFTFGLSLVKLDIRQESERHTDVIDAITTHLGIGSYRE
480 WPEDKRQEWWSELRGKRPLLPDPQTDEIADVIGHVLAELPPDSFGPYIISMATAP
540 SDVLAVELLQRECGVRQPLPVVPLFERLADLQSAPASVERLFSDWYMDRIKGKQQVMVG
600 YSDSGKDAGRLSAAWQLYRAQEEMAQVAKRYGVKLTLFHGRGGTVGRGGGPTHLAILSQP
660 PDTINGSIRVTVQGEVIEFCFGEELCFQTLQRFTAATLEHGMHPPSPKPEWRKLMDEM
720 AVVATEEYRSVVVKEARFVEYFRSATPETEYGRMNIGSRPAKRRPGGGITTLRAIPWIFS
780 WTQTRFHLPVWLGVAAFKFAIDKDVRNFQVLKEMYNEWPFFRVTLDLLEMVFAKGDPGI
840 AGLYDELLVAEELKPGKQLRDKYVETQQLLQIAGHKDILEGDPFLKQGLVLRNPYITT
900 LNVFQAYTLKRIRDPNFKVTPQPLSKEFADENKPAGLVKLNPASEYPPGLEDTLILTMK
960 GIAAGMQNTGA
```

## Protein sequence documentation

- [protein-sequence\(\)](#)

### protein-sequence

Display a protein sequence in a block with amino acid numbering

#### Parameters

```
protein-sequence(
    line-length,
    protein
) -> content
```

#### line-length

The maximum length of amino acid to display in a line. **Optional**.

Default: **50**

#### protein

Amino acid sequence (one letter code) of the protein to display

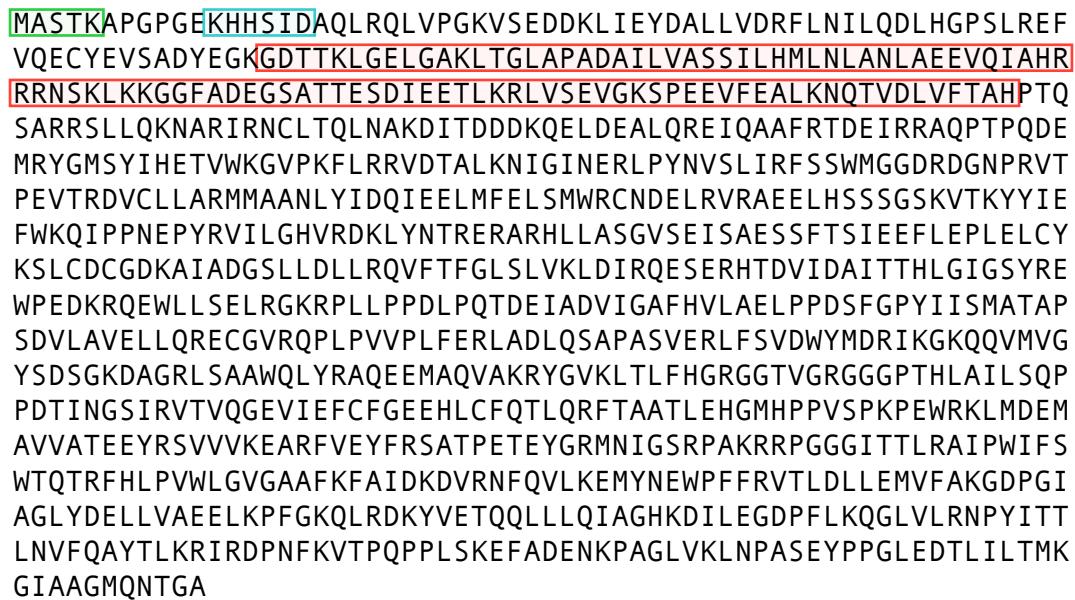
## Protein diagram

This figure is based on the [fletcher](#) package features.

### Example :

```
#import "@preview/proteograph:0.2.1": *  
  
#let tint(c) = (stroke: c, fill: rgb(..c.components().slice(0,3), 5%), inset: 1pt)  
  
#protein-diag(line-length: 60,  
"MASTKAPGPGEKHHSIDAQLRQLVPGKVSEDDKLIEYDALLVDRFLNILQDLHGPSLREFVQECEVSADYEGKDTTKLGELGAKLTGLAPADAILV  
(pos: (1,5), style: tint(green)),  
(pos: (12,17), style: tint(teal)),  
(pos: (75,177), style: tint(red)),  
)
```

### Result :



MASTKAPGPGEKHHSIDAQLRQLVPGKVSEDDKLIEYDALLVDRFLNILQDLHGPSLREFVQECEVSADYEGKDTTKLGELGAKLTGLAPADAILV  
RRNSKLKKGGFADEGSATTESDIEETLKRLVSEVGKSPEEVFEALKNQTVSDLVFTAHTPQ  
SARRSLLQKNARIRNCLTQLNAKDITDDDQELDEALQREIQAAFRTEIRRAQPTPQDE  
MRYGMSYIHETVKGVPKFLRRVTALKNIGINERLPYNVSLIRFSWMGGDRDGPNPRVT  
PEVTRDVCLLARMMAANLYIDQIEELMFELSMWRCNDELRVRAEELHSSSGSKVTKYYIE  
FWKQIPPNEPYRVLGHVRDKLYNTRERARHLLASGVSEISAESSFTSIEEFLEPLECY  
KSLCDCGDKAIADGSLLDLLRQVFTFGLSLVKLDIRQESERHTDVIDAITTHLGIGSYRE  
WPEDKRQEPLLSELRGKRPLLPPDLPQTDEIADVIGAFHVLAELPPDSFGPYIISMATAP  
SDVLAVELLQRECGRVQPLPVVPLFERLADLQSAPASVERLFSVDWYMDRIKGKQQVMVG  
YSDSGKDAGRLSAAWQLYRAQEEMAQVAKRYGVKLTLFHGRGGTVGRGGGPTHLAILSQP  
PDTINGSIRVTVQGEVIEFCFGEEHLCFQTLQRFTAATLEHGMHPPVSPKPEWRKLMDEM  
AVVATEEYRSVVVKEARFVEYFRSATPETEYGRMNIGSRPAKRRPGGGITTLRAIPWIFS  
WTQTRFHLPVWLGVGAASFKAIDKDVRNFQVLKEMYNNEWPFFRVTLDLLEMVFAKGDPGI  
AGLYDELLVAEELKPGKQLRDKYVETQQLLLQIAGHKDILEGDPFLKQGLVLRNPYITT  
LNVFQAYTLKRIRDPNFKVTPQPPLSKEFADENKPAGLVKLNPASEYPPGLEDTLILTMK  
GIAAGMQNTGA

## Protein diagram documentation

- [protein-diag\(\)](#)

### protein-diag

Display a protein sequence in a block with amino acid numbering

#### Parameters

```
protein-diag(  
    line-length: int,  
    boxes: array,  
    protein: str,  
    ..box: dictionary  
) -> content
```

**line-length** int

The maximum length of amino acid to display in a line. **Optional**.

Default: 50

**boxes** array

Array of boxes to draw in the protein sequence **Optional**.

This can be used to visualize the position of one or more peptides

example for 3 peptides :

((pos: (1,5), style: tint(green)),(pos: (12,17), style: tint(teal)),(pos: (75,177), style: tint(red)))

Default: ()

**protein** str

Amino acid sequence (one letter code) of the protein to display

**.box** dictionary

box item to draw in the protein sequence **Optional**.

This can be used to visualize the position of one or more peptides

example :

(pos: (1,5), style: tint(green))

```
1 #import "@preview/  
proteograph:0.2.1": * typ  
2 #protein-diag(line-length: 60,  
3 "MASTKAPGPGEKHHSIDAQLRQLV",  
4 (pos: (1,5), style: (stroke: red,  
inset: 1pt)),  
5 (pos: (12,17), style: (stroke: teal,  
inset: 3pt))  
6 )
```

MASTKAPGPGEKHHSIDAQLRQLV

## Isotope pattern plot

**Example :**

```
#import "@preview/proteograph:0.2.1": *
```

```
#isotope-pattern-plot(  
mz:(792.89009986061, 793.3914387289032, 793.8927444414951),  
intensity:(22000, 18000, 8000),  
th-ratio: ( 0.4182709626684006, 0.3428843140088085, 0.157722041765769),  
color: orange,  
)
```

**Result :**

