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Proteograph, typst package for proteomics data visualization directly from JSON

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Typst

[Typst](#)¹ is a new, free and open-source markup-based typesetting system for scientific publications, written in Rust. It is designed to provide an alternative to both advanced tools, such as LaTeX, and simpler tools, such as Word and Google Docs. Typst allows you to produce high-quality scientific documents in PDF, SVG or HTML format for your slideshows, posters, articles or books.

Typst's syntax is simple and similar to Markdown, yet it is also powerful and extendable through a wide variety of [packages](#).

[Proteograph](#)² is a Typst package that adds the ability to generate proteomics figures directly in your documents.

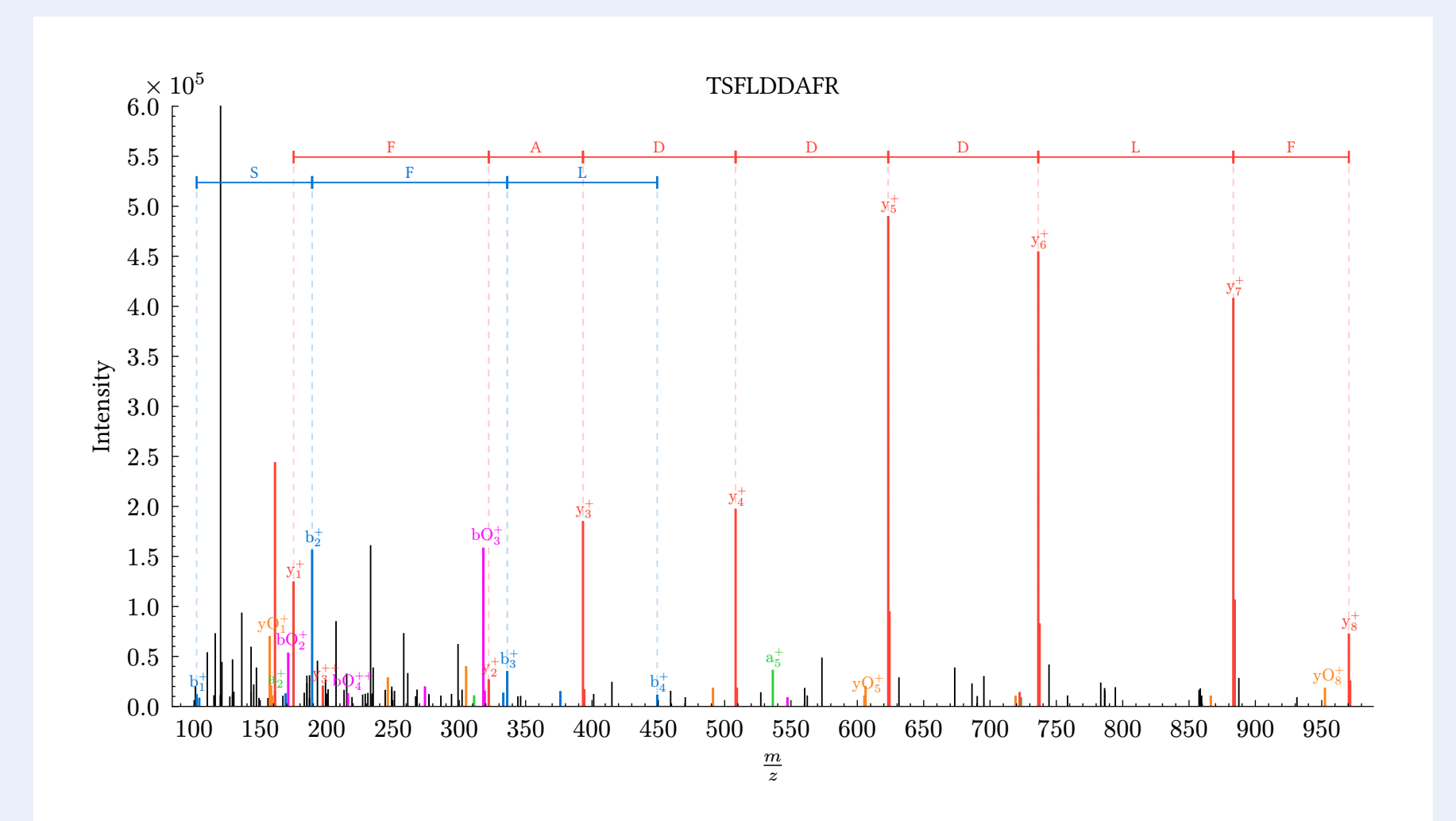
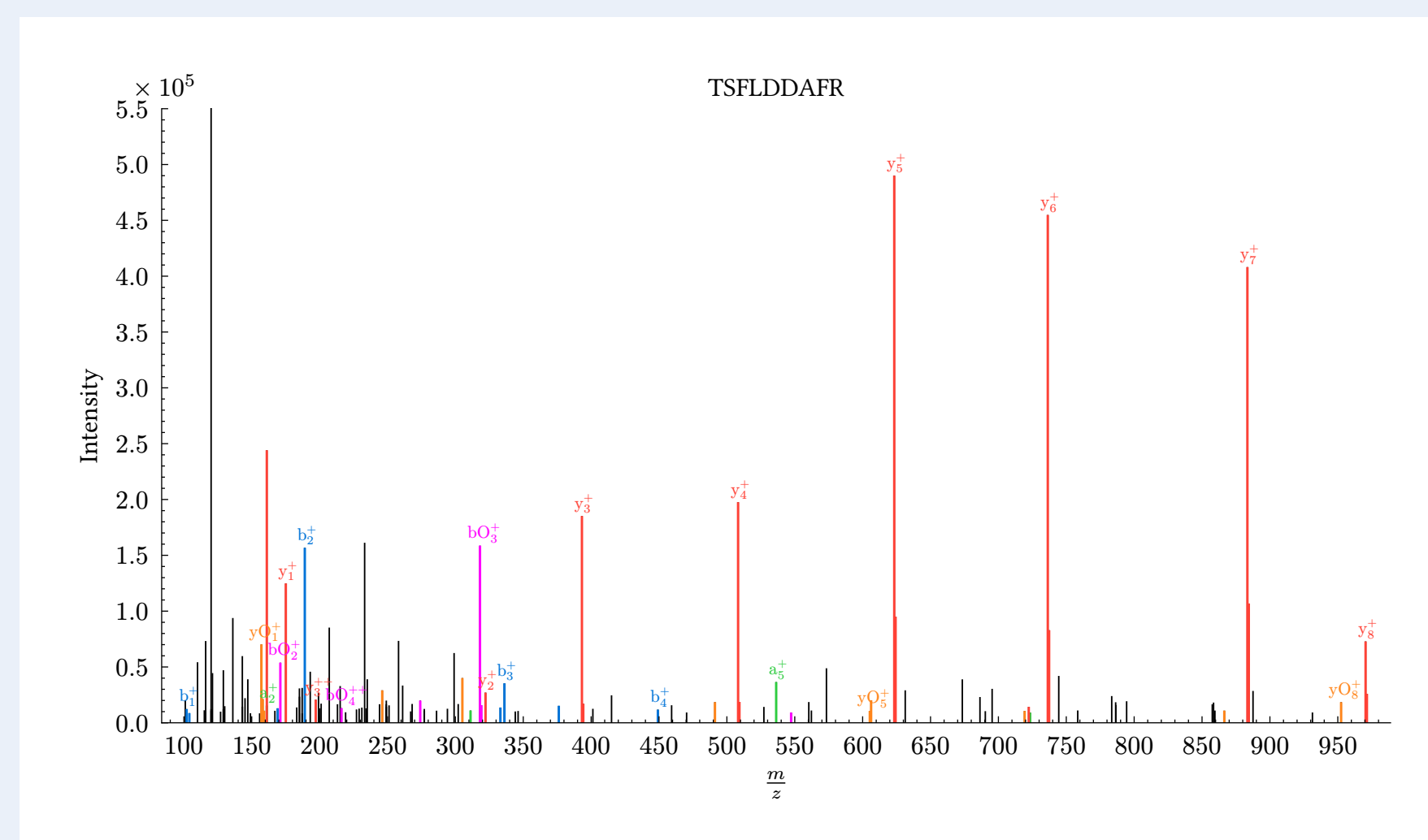
Proteograph is a GPLv3 project. The source code is available on Codeberg, and Proteograph is shipped with Typst as an official "universe" package. Thus, invoking "proteograph" in your Typst document is sufficient to start using it.

Data source ProteoBench project, DDA precursor quantification (QExactive) module.

¹ <https://typst.app/>

² <https://typst.app/universe/package/proteograph/>

Annotated MS/MS spectrum



On the left Annotated MS/MS spectra for the peptide sequence TSFLDDAFR. JSON data contains peaks (mz + intensities) and matching ions positions. This file can be produced using [i2MassChroQ](#)¹.

On the right The same annotated with additional manual annotation to highlight given mass delta between peaks.

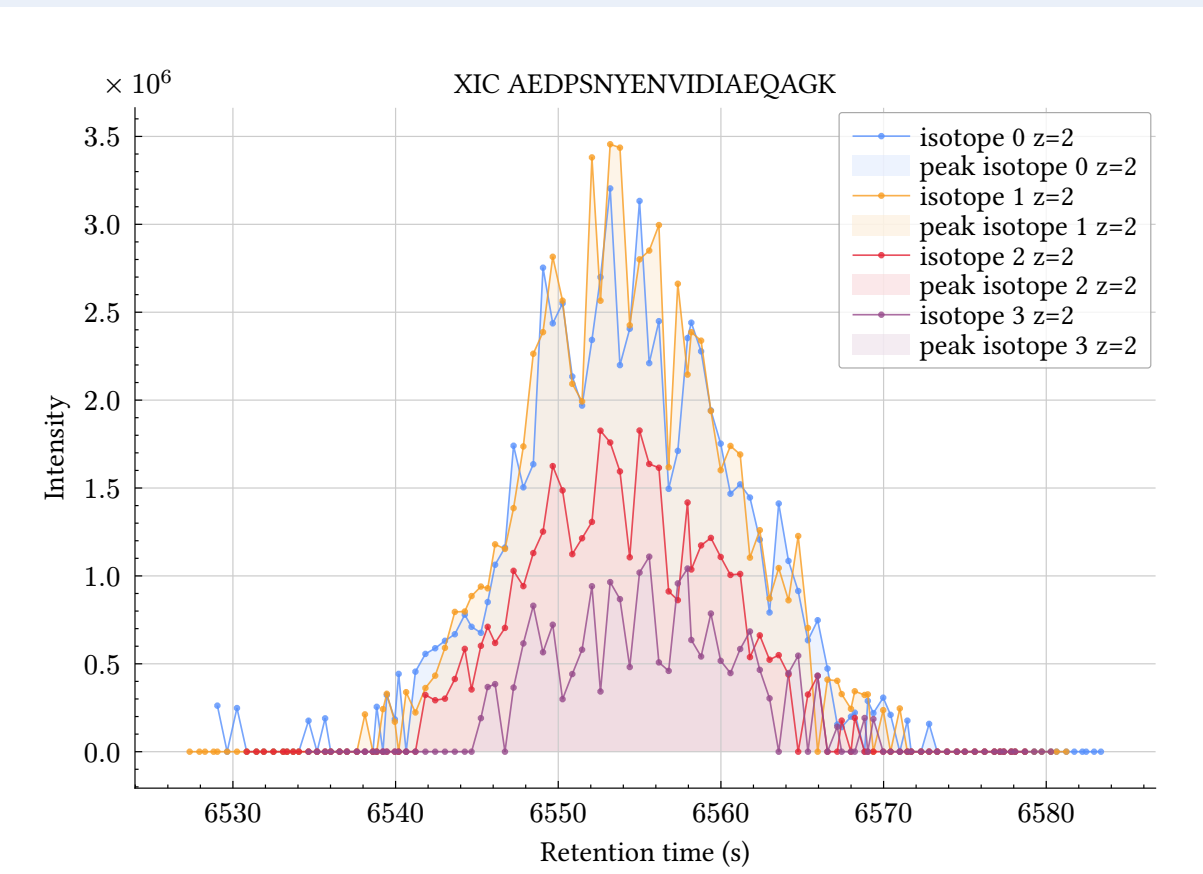
```
#import "@preview/proteograph:0.2.1": *
#let complete_psm = json("../data/pepa1c141_LFQ_Orbitrap_DDA_Condition_B_Sample_Alpha_03_92636.json")
#ms2spectra-plot(max-intensity: 550000, width: 20cm, height: 10cm, title: complete_psm.proforma, spectra:
complete_psm.spectra, ion-series: complete_psm.ion-series)
```

¹ [1] O. Langella *et al.* "Full Native timsTOF PASEF-Enabled Quantitative Proteomics with the i2MassChroQ Software Package," *Journal of Proteome Research*, vol. 23, no. 8, pp. 3353–3366, Aug. 2024, doi: [10.1021/acs.jproteome.3c00732](https://doi.org/10.1021/acs.jproteome.3c00732).

eXtracted Ion Chromatogram

The "xic-plot" function displays ion chromatograms with full visualisation of the isotope pattern. This graphic is useful to control the reliability of the peptide quantification.

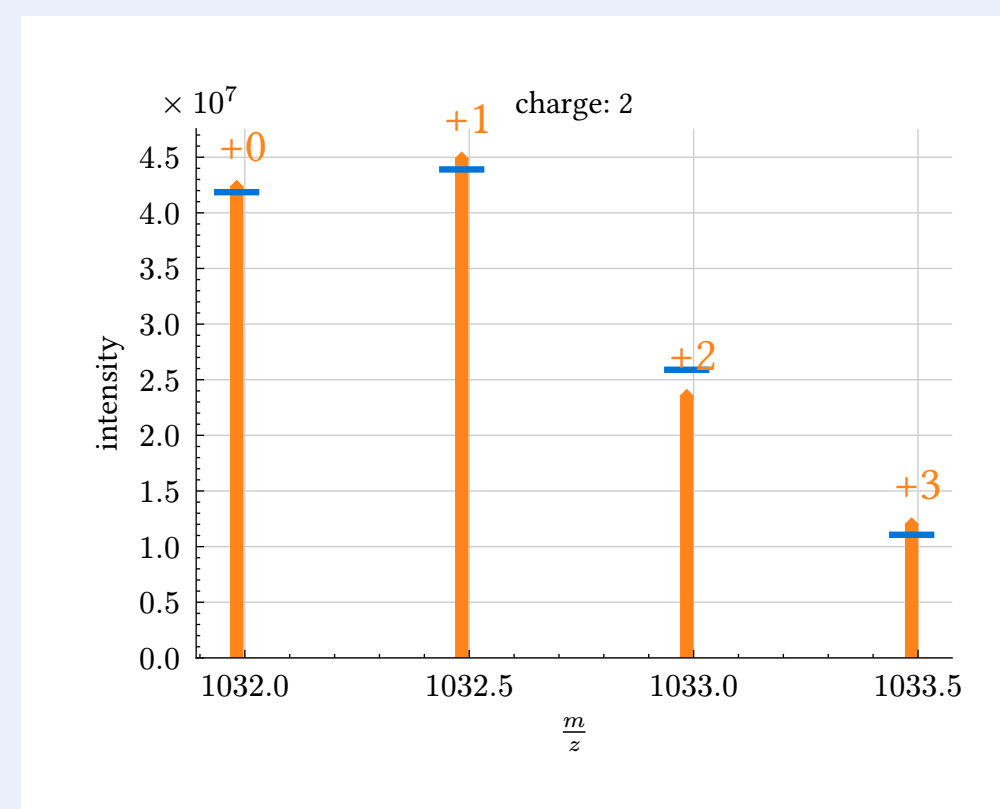
The JSON input contains the ion metadata and a partial chromatogram at this retention time (see the [Proteograph documentation](#) for more information). This can be produced by MassChroQ3, which is embedded in [i2MassChroQ](#).



```
#import "@preview/proteograph:0.2.1": *
#let xic-trace = json("../data/xic_pepb14a3_z2.json").quantification_data
.pepb14a3.first()
#xic-plot(height: 10cm
title: "XIC "+xic-trace.proforma,
..get-xic-data(xic-trace, type: "trace"))
```

Using the same dataset, the "isotope-pattern-plot" function allows you to compare the intensities of the measured isotopic mass areas with the theoretical ratios.

Orange Measured areas under the curve
Blue bar Expected theoretical abundance

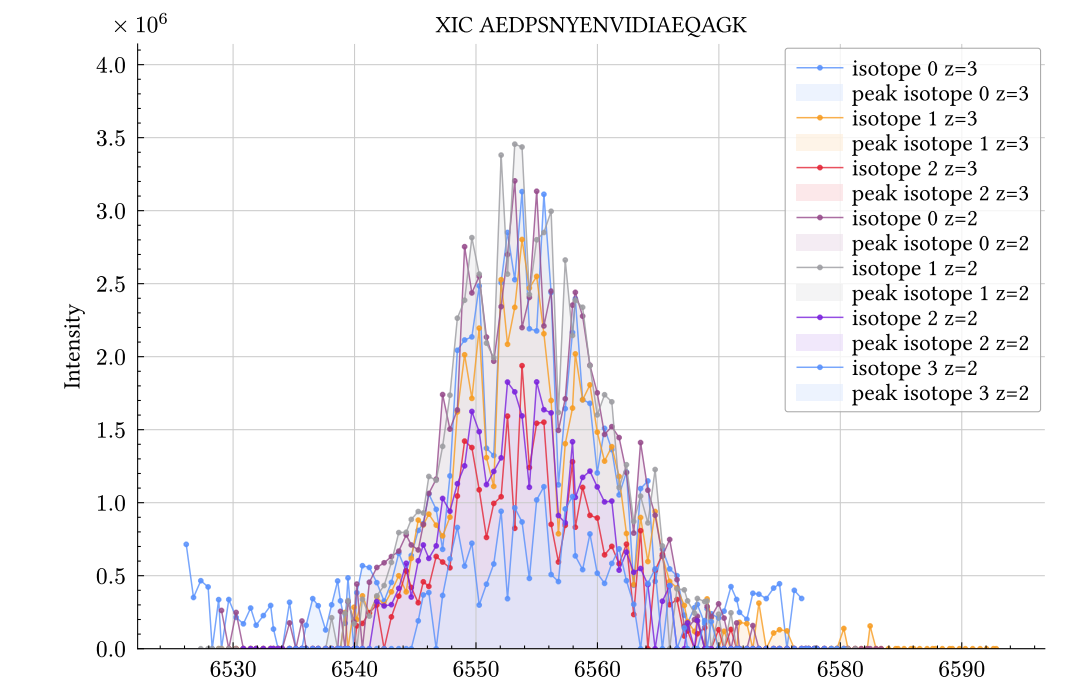


```
#import "@preview/proteograph:0.2.1": *
#let peptide_measures = json("../data/xic_pepb14a3_z2.json")
.quantification_data.pepb14a3.first()
#isotope-pattern-plot(legend: none,height: 7cm,
width: 10cm,
..get-isotope-pattern-data(peptide_measures,
charge: 2))
```

A complete report with automatic layout can be generated for a set of peptides/proteins (see beside).

pepb14a3 in msrun1

```
ipeptide:pepb14a3.msrun1.msrun1.pepb14a3.msrun1
LFQ:MS1:MS2:DDA_Condition_A_Sample_Alpha_03.msrun1
AEDPSNVNVDIAEQAGK modk: [C 87 11 136 0 35 N 23 S 0]
targeted retention time: 6548.0574
isotope 0   isotope 1   isotope 2   isotope 3
me: 654.32544   me: 656.01794   me: 658.09217   me: 660.32038
charge: 2     charge: 2     charge: 2     charge: 2
th ratio: 0.32   th ratio: 0.34   th ratio: 0.2   th ratio: 0.09
mz range: 648.317-   mz range: 658.051-   mz range: 658.985-   mz range: 659.519-
658.331           658.665           658.999           659.333
quality: 100     quality: 100     quality: 100     quality: 100
area: 38114252    area: 34211852    area: 30262184    area: 25262184
isotope 0   isotope 1   isotope 2   isotope 3
me: 1032.0182   me: 1033.83827   me: 1035.96462   me: 1038.0879
charge: 2     charge: 2     charge: 2     charge: 2
th ratio: 0.32   th ratio: 0.34   th ratio: 0.2   th ratio: 0.09
mz range: 1031.972-   mz range: 1032.473-   mz range: 1032.974-   mz range: 1033.475-
1032.192         1032.494         1032.995         1033.496
quality: 100     quality: 100     quality: 100     quality: 100
area: 42319119    area: 48675809    area: 23335985    area: 11931815
```



```
#import "@preview/proteograph:0.2.1": *
#let all-peptide-data = json("../data/xic_pepb14a3.json")
#mcqjson-report-peptide-measures(all-peptide-data,
peptide-id: "pepb14a3")
```

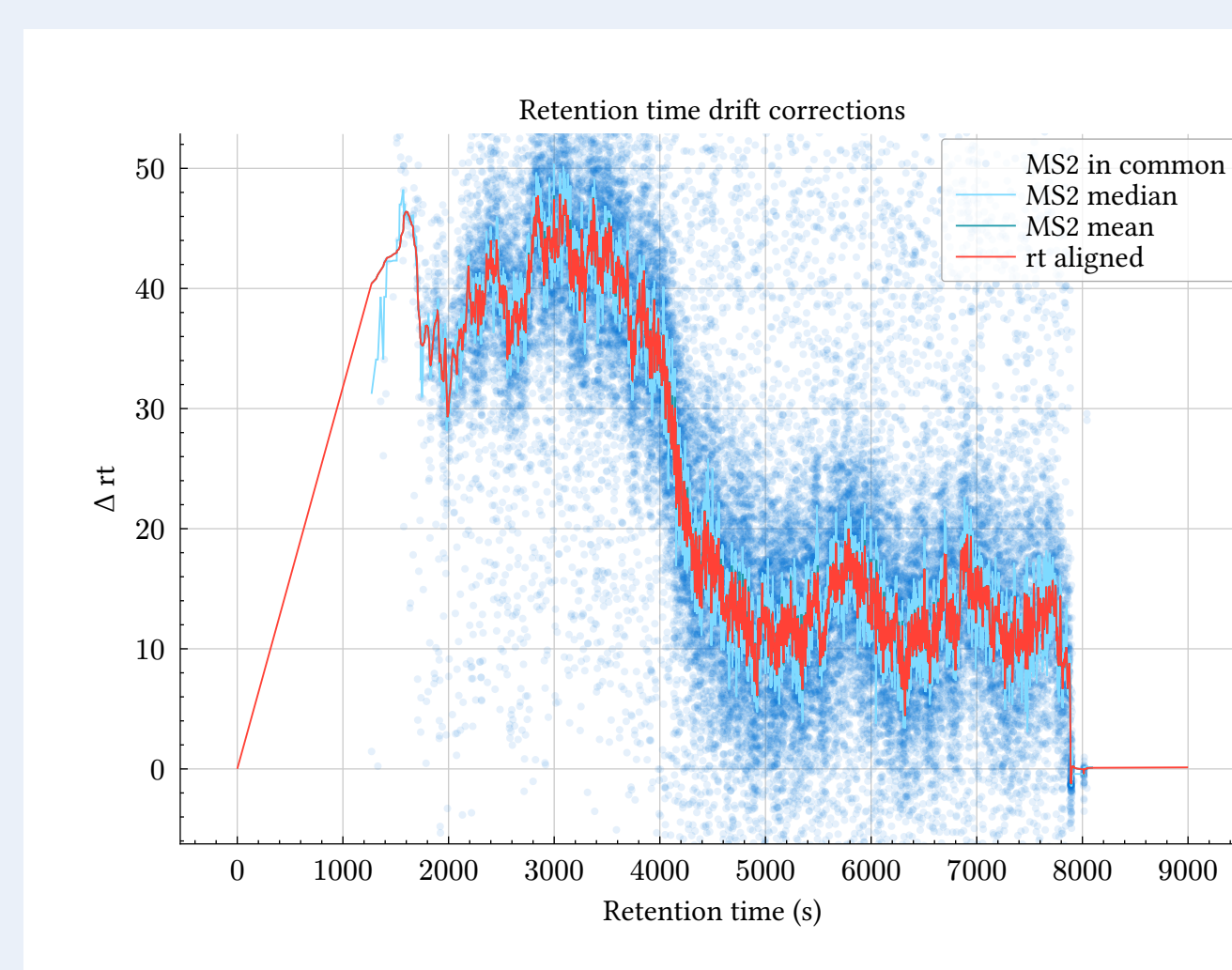
Protein diagram

This simple function displays a protein sequence and highlights peptides using start and stop positions.

```
MSEPGGGGGEDGSAGLEVSANQVADVSLATEFIMNEYKDRKTRITRSLDDAFKRLNES
ALRFGNPLLVQDVEYTPVLPVLRVRRVTRGRVLTLLGQDDILSPSFVIFLSTRDPT
VEFPDLCRVTFVNFVTRKSLQSCLELVKAEKRPVDEKSDLLKQGEFLRLRQL
EKSLQALNEVKRILDDDTIITLLENKREAEVTRKVEEDIVMQEVTVSQYLLPLS
TACSSIFFTMESLKQHFHYQSLQFFLDIYHNVLYENPNLKGVTQHTQRLSIIITKDLFQ
VAFNRVARGHLHQDHITFAHLRLARLKLKGTVEPTVDAEFQHLRONEIVLSAGSTPRIQ
GLTYEQEAVRSLCPAPRDLIAVQVADQFQWLDSSSEPTVYVYVSEETPATIGQ
AIHRLLLIQAFRDRDLAMAHMFVSTNLGSEFMSMEQPLDLTHIVGTEVPNTVLMCS
VPGYDAGHVEDLAAEQNTQITSIAGSAGFNQADKINTAVKSGRNVMLKNVHLPAGW
LMLKELKHLISQPHACFRFLFTEINPKVFNLLKAGRIFFVFPFQVKNMLRTFS51P
VSRICKSPNEARLRYFLAWFMAITQERLRYAPLQNSKRYEFGESDLSACDQVTLDD
TAKGRQNI SPDKIPMSALKITLMAQSIYGGRVDFDRLNLTFLERLFTFRSDFSEFKLA
CKVDGHDIQMPDGRREEFQVQVELLPTDTQPSWLGLPNNAERVLLTQGVNHSKMLK
MQLLEDEDDLAYAEKTKTRTSTSDGRPAWRLHTTASNWLHL1PQTLSHLKRVTENI
KDFLFFEREVWNGKLLQDQRLADVQVQEGKQKQVYVRLTINLWGLIPSWIS
HYTPAGMTVIQHVDFSEIRIKQLQISLAASGGAKELKNIHVCLGGLVPEAVYIATR
QYVAQANSLSLEELLENVTTSGATLDACDFVGTGLKQATCNKLSLSNAISTAL
PLTQLRWQNTENKASVVTLPVYLFNTRADLIFVDFEATJAE
```

```
#protein-diag(line-length: 60,
"MSEPGGGGGEDGSAGL...",
(pos: (47,55), style: tint(red)),
(pos: (154,161), style: tint(teal)),
(pos: (533,546), style: tint(teal)),
(pos: (1030,1035), style: tint(teal)),
)
```

Retention time alignment



```
#import "@preview/proteograph:0.2.1": *
#let rt_align = json("../data/proteobench_alignment.json").alignment_data[0].alignment.corrections.msrun1
#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)
```

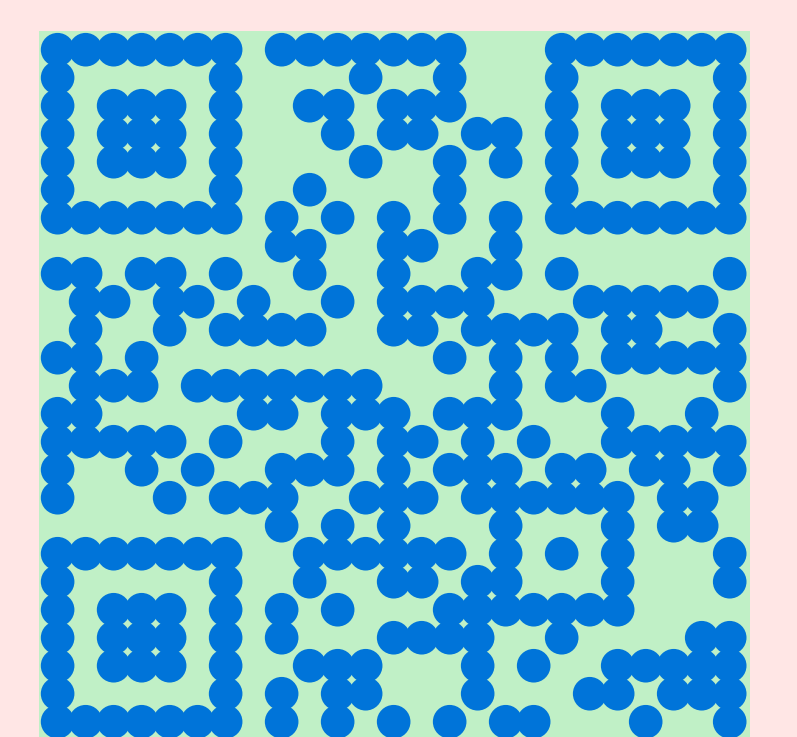
Aligning the retention times between MS runs is critical to achieving the best possible MS1 quantification.

This plot uses MassChroQ3 data to visualise the shift in retention time during chromatography between two ms runs.

Resources

Scan this QR code to download the poster containing all the clickable links.

The full documentation, JSON data file examples and code snippets are available in the [Codeberg repository](#)¹.



¹ <https://codeberg.org/olangella/proteograph>