161128 EXP16 EMbuffer samples

QC Metrics reported by Progenesis QI for proteomics v3.0.5995.47167
Date: 06-Dec-2016 at 13:26
Experiment design: Grouping

This QC report contains **all metrics** for the experiment named above.

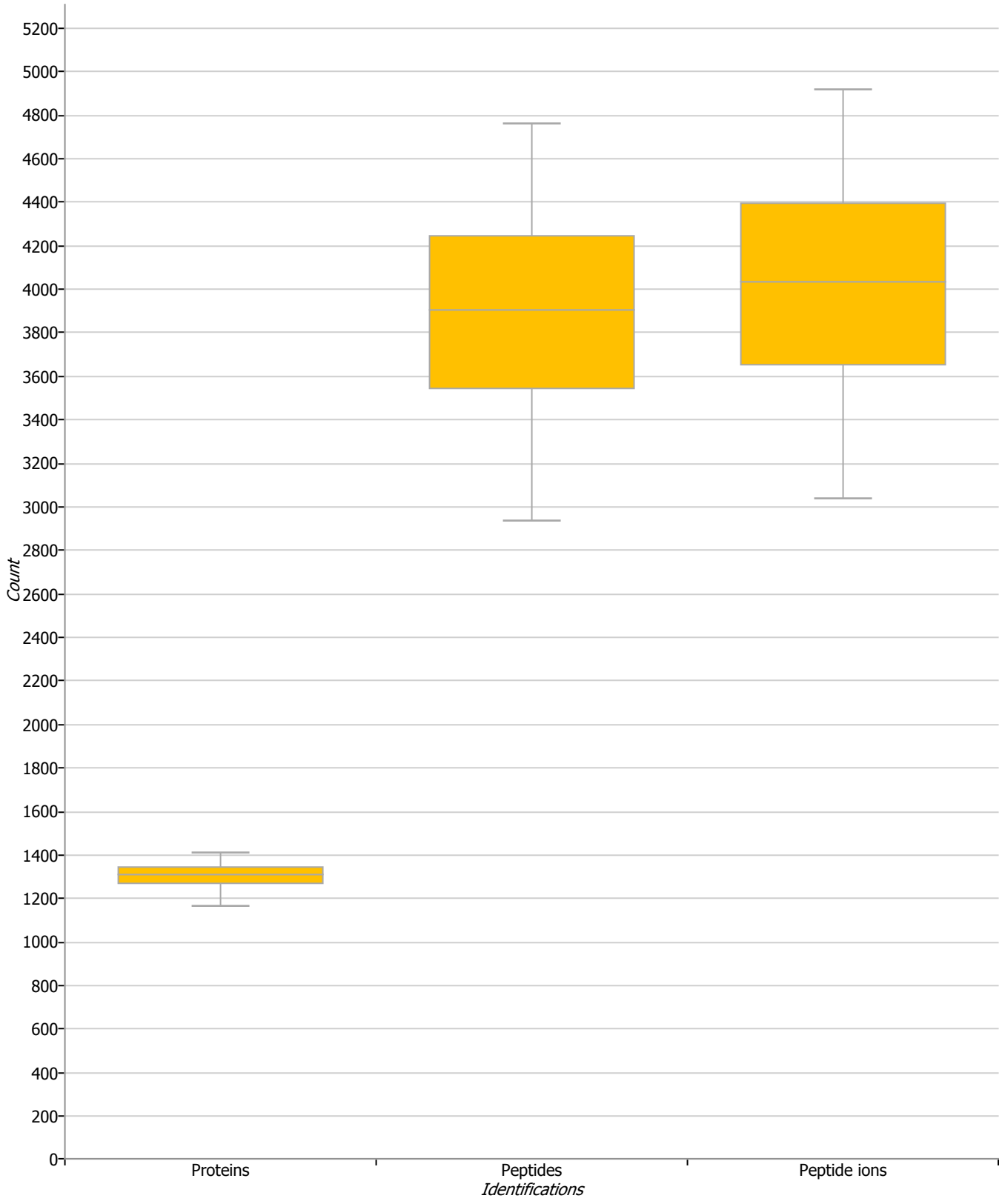
Reported metrics

0 of the 19 metrics reported have been manually flagged for attention.

- Identifications overview
- LC peak width
- Peptide ion dynamic range
- Precursor m/z
- Precursor retention time
- Mass errors
- Precursor charges
- Missed cleavages (assuming trypsin)
- Peptides per protein (overview)
- Modifications
- Missed cleavages
- Abundance dynamic range
- Mass accuracy
- Scan rates
- Proteins
- Peptides
- Peptides per protein (by condition)
- Percentage of peptide ions identified
- Protein overlap

Identifications overview

The chart below provides the number of identifications per run by category. Data are plotted for all runs in the current experiment design. The box represents the interquartile range and the whiskers the maximum and minimum.

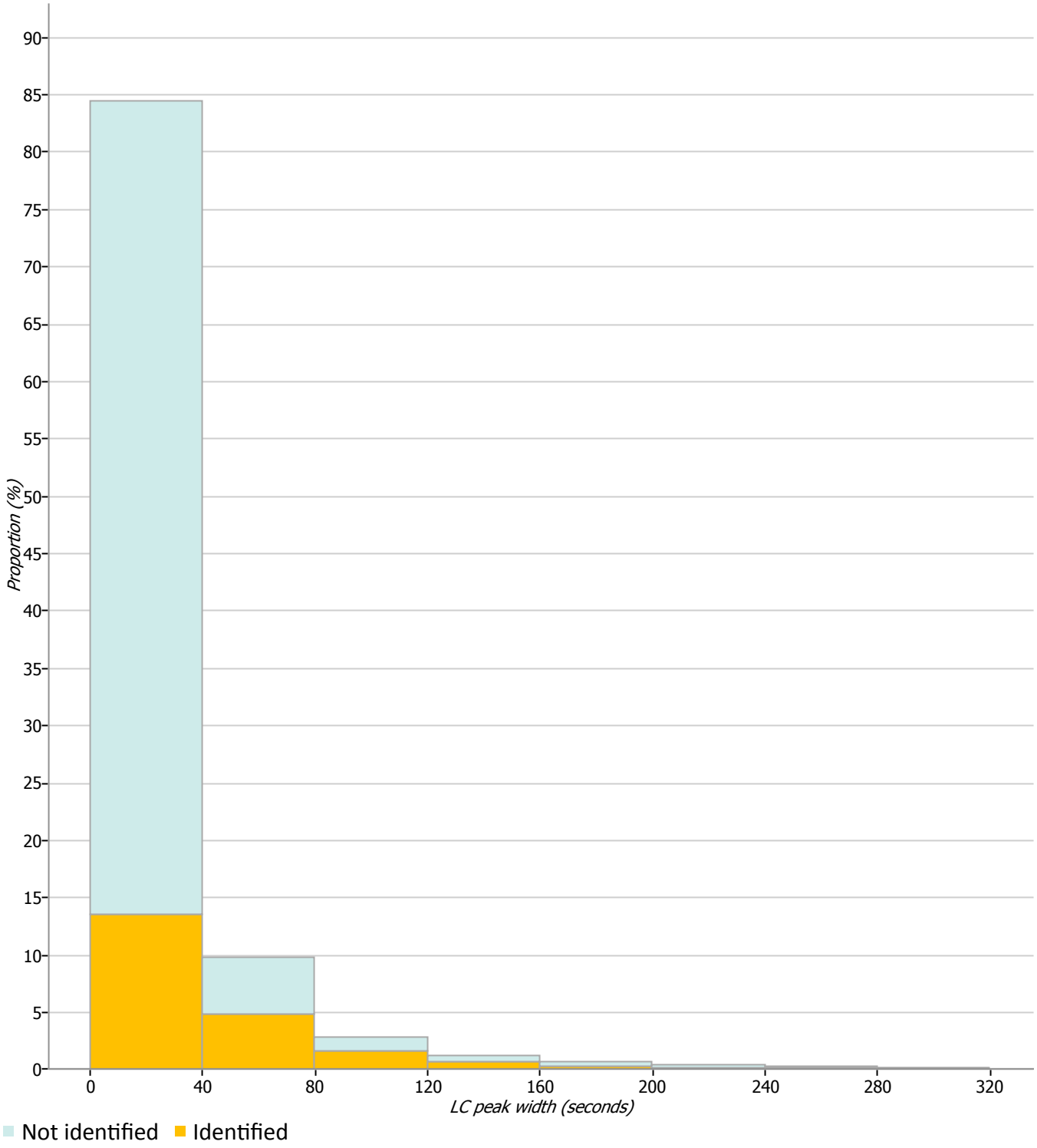


LC peak width

This chart shows the proportional distribution of peak widths in retention time, for all the detected peptide ions in the experiment. Widths are binned into categories for simple comparison. Identified peptide ions are shown in yellow.

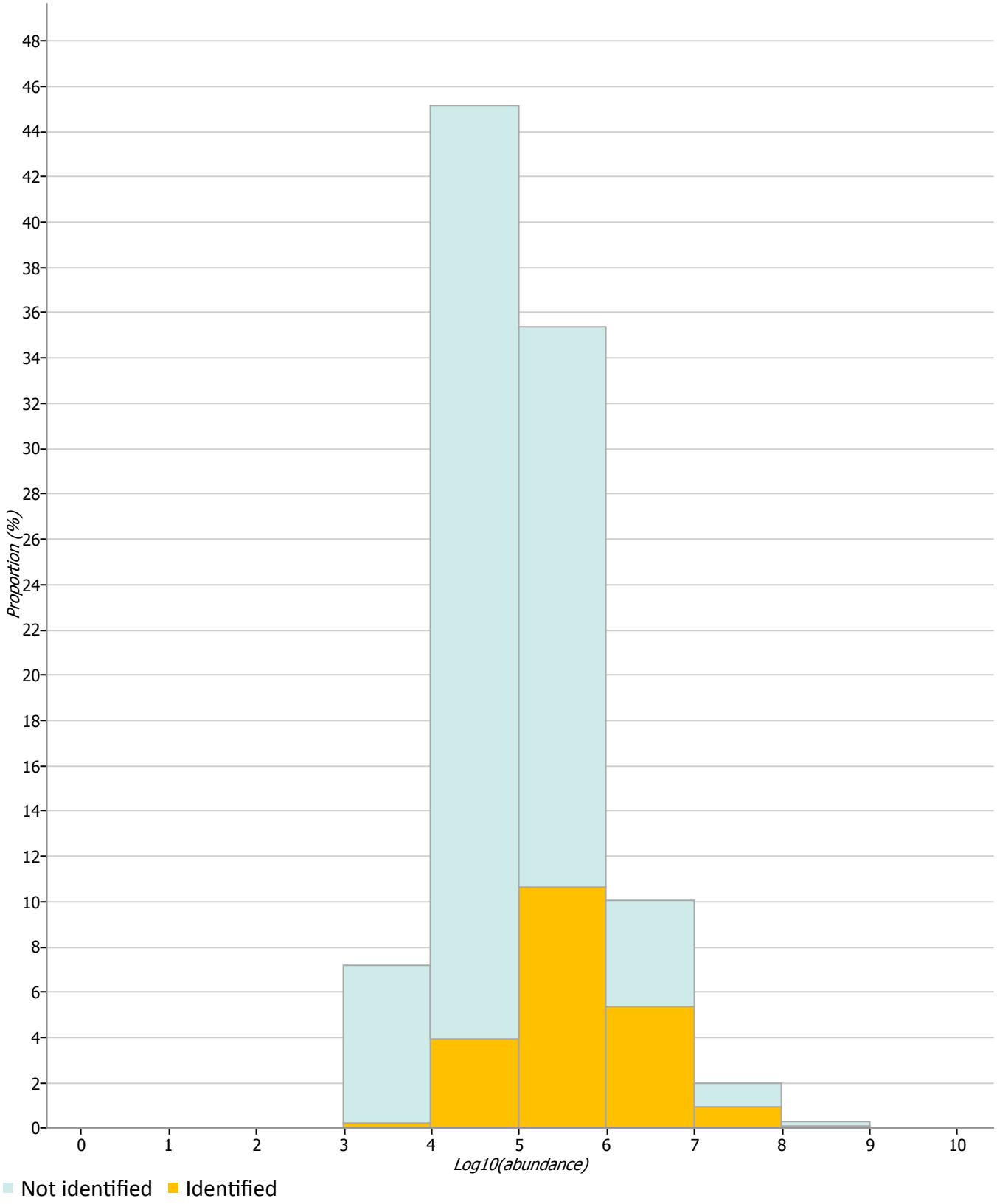
Potential problems:

- A peak width that is different from that expected for your setup may indicate a problem with the chromatographic separation.



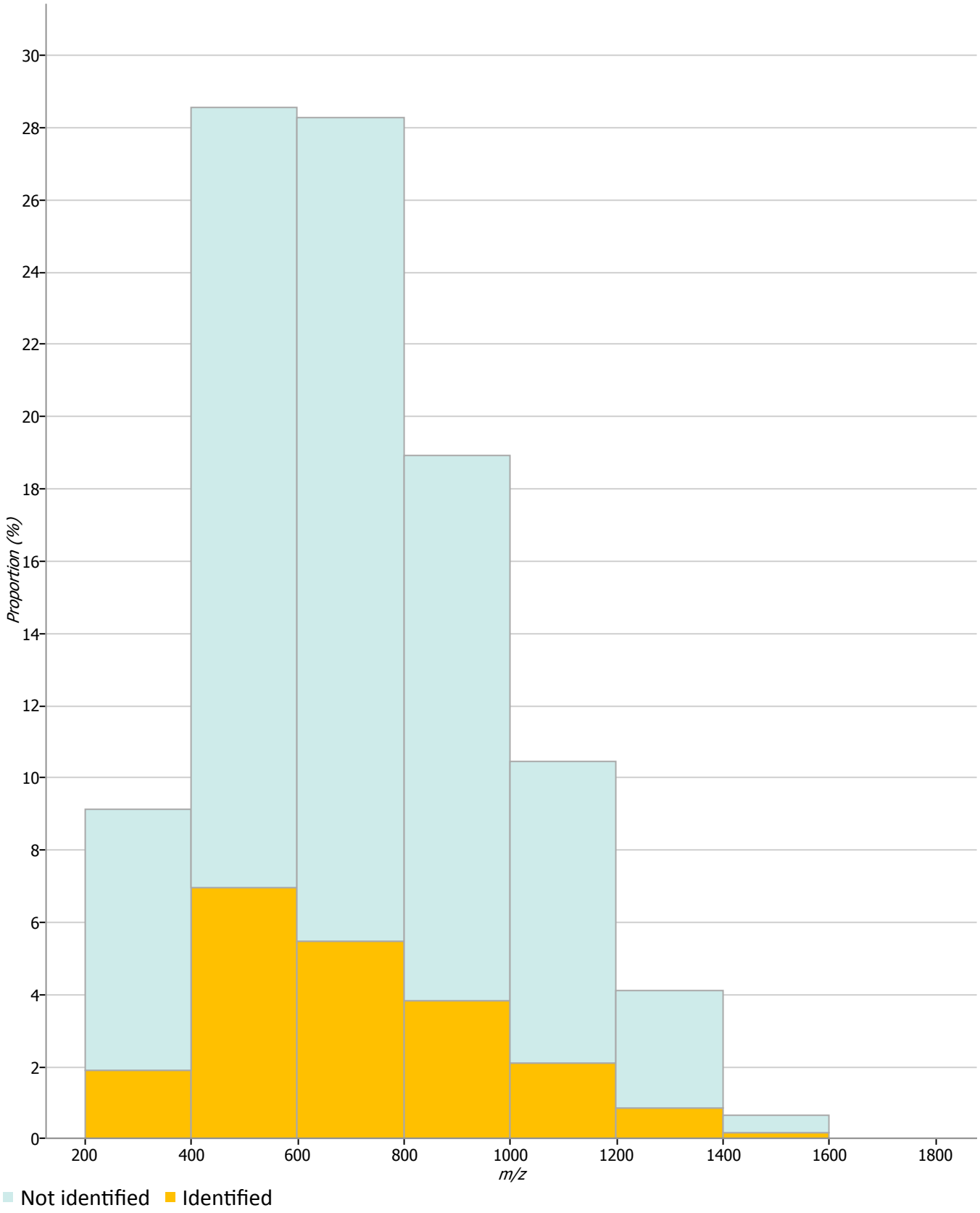
Peptide ion dynamic range

This chart shows log abundance for peptide ions, calculated using the current experiment design. Each peptide ion is assigned its abundance based on the highest mean value for any condition's runs. Data are binned and shown as a proportion. Identified peptide ions are shown in yellow.



Precursor m/z

This chart shows the distribution of m/z values for all peptide ions in the experiment. Identified peptide ions are shown in yellow.

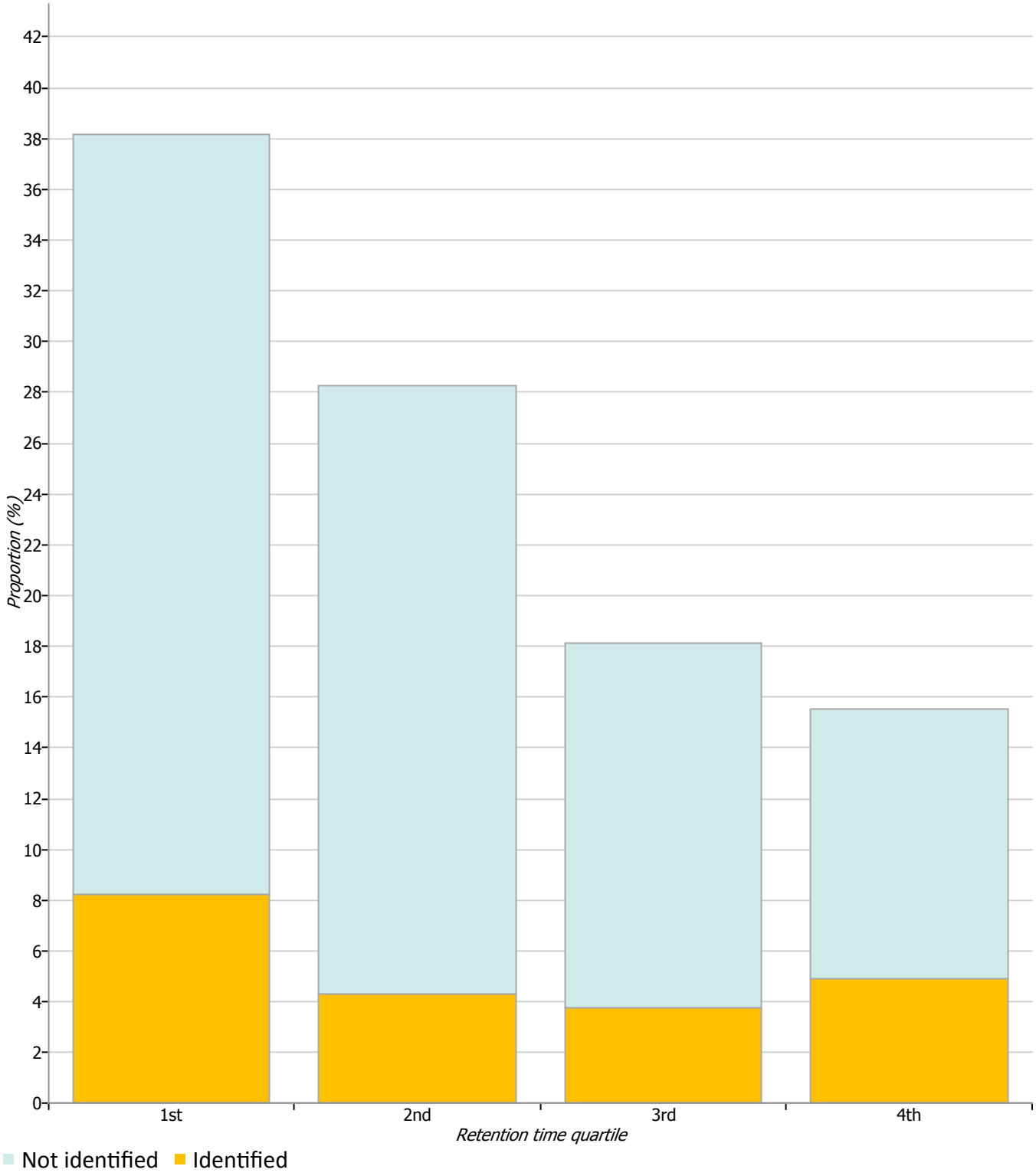


Precursor retention time

This chart shows the proportion of precursor peptide ions eluting into each quartile of the LC run. Identified peptide ions are shown in yellow.

Potential problems:

- A majority of peptide ions eluting at the start or end of the run may indicate problems with the chromatographic separation or that the setup is not ideal for a successful separation.

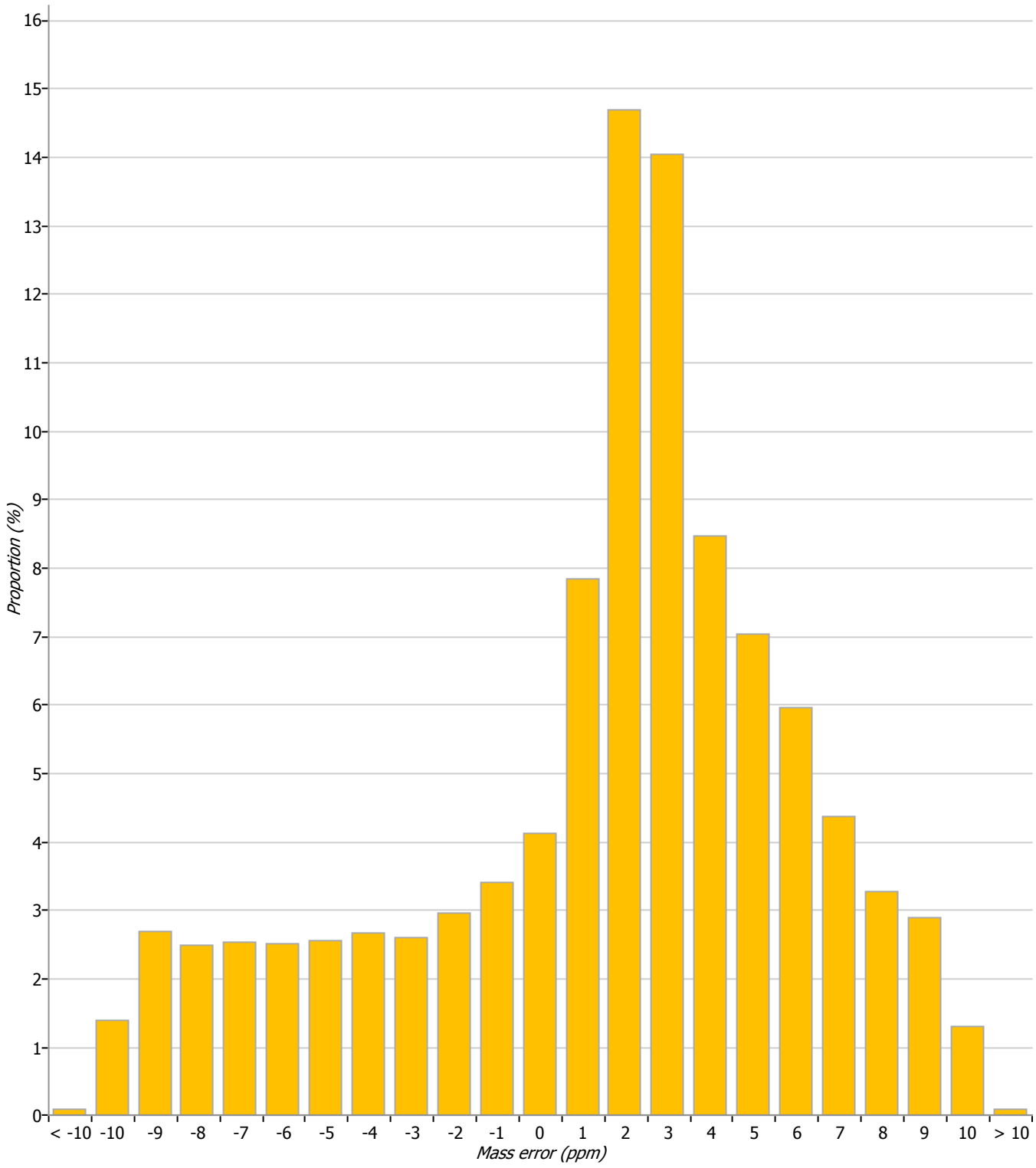


Mass errors

This chart shows the mass error calculated for identified peptide ions. The proportion of peptide ions with a given binned error value is plotted. For a more detailed plot, see the *Mass accuracy* metric.

Potential problems:

- A larger than expected spread could indicate that search parameters are too lenient.
- A bias of the peak from zero ppm could indicate instrument bias.

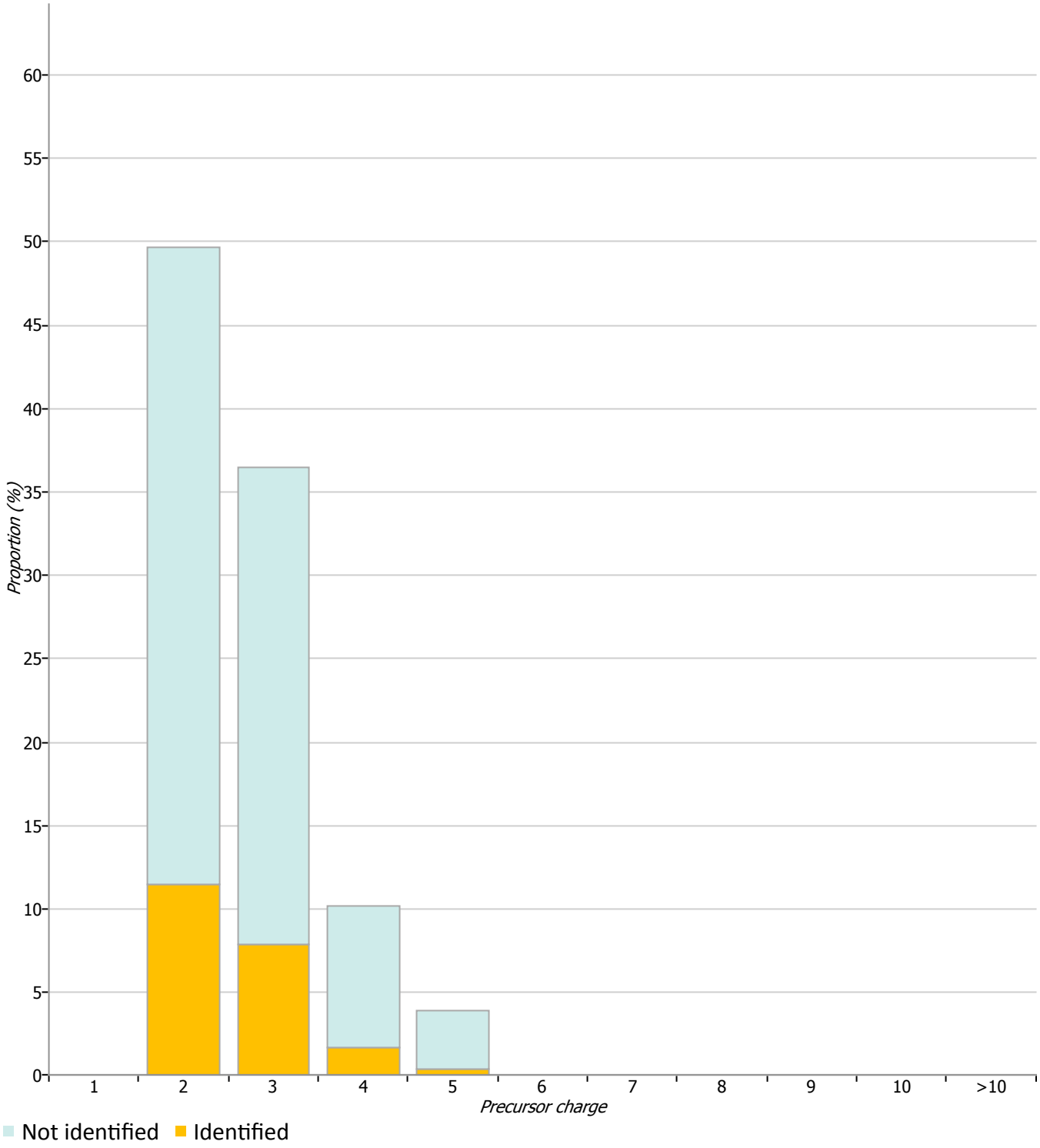


Precursor charges

This chart shows the percentage of peptide ions with various charge states.

Potential problems:

- A skew towards low charge peptide ions may indicate poor ionisation, suggesting that you may need to raise the collision voltage.
- A skew towards high charge peptide ions may indicate excessive ionisation, suggesting that you may need to lower the collision voltage.

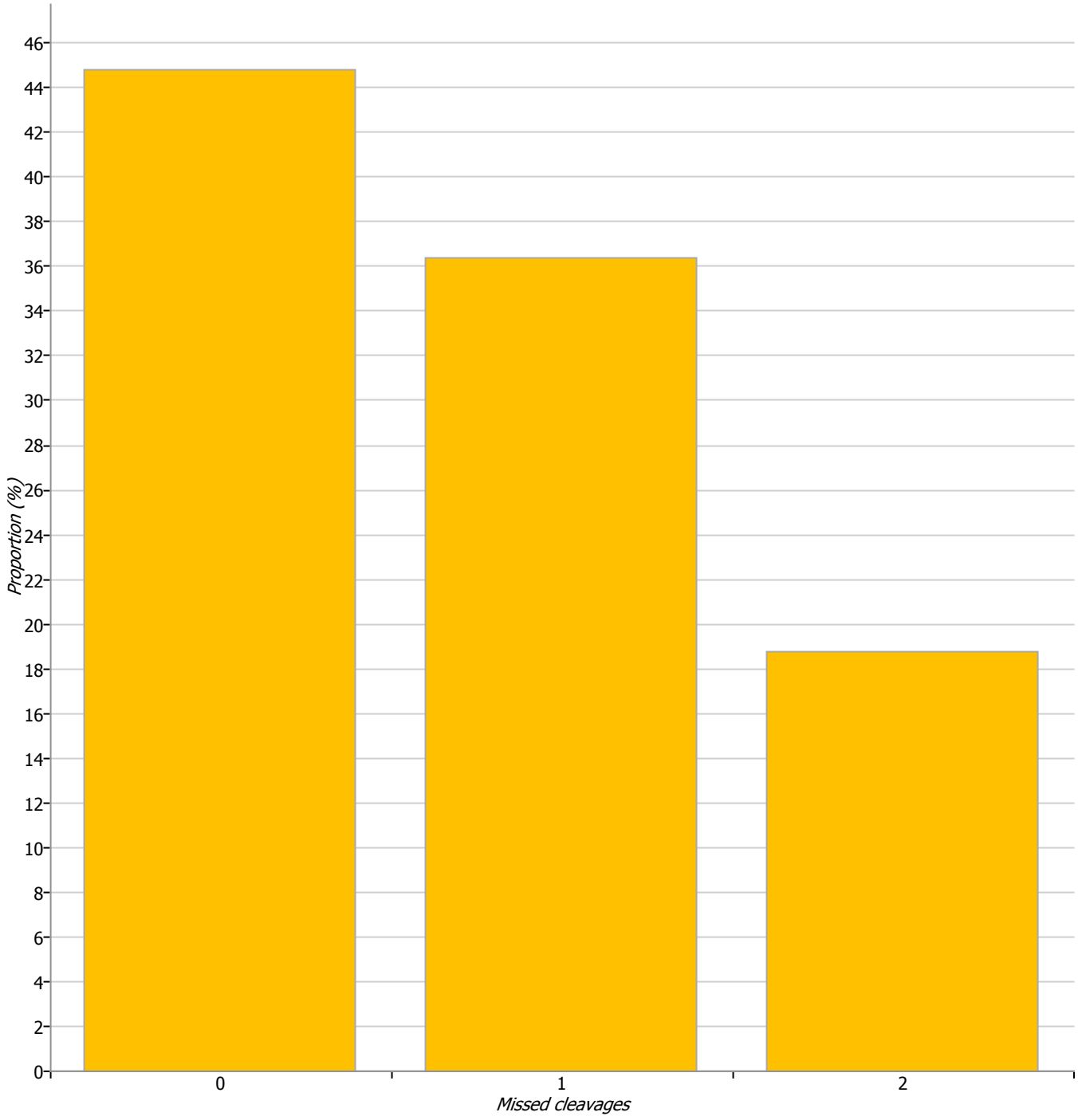


Missed cleavages (assuming trypsin)

This chart shows the distribution of missed cleavages per identified peptide ion across the whole experiment, assuming the proteins were treated with trypsin and using each peptide ion's highest scoring identification. For an alternative visualisation showing the data subdivided by experimental condition, see the *Missed cleavages* metric.

Potential problems:

- A high proportion of missed cleavages may indicate problems in trypsinization.
- An absence of missed cleavages may indicate that the database search parameters were too stringent.

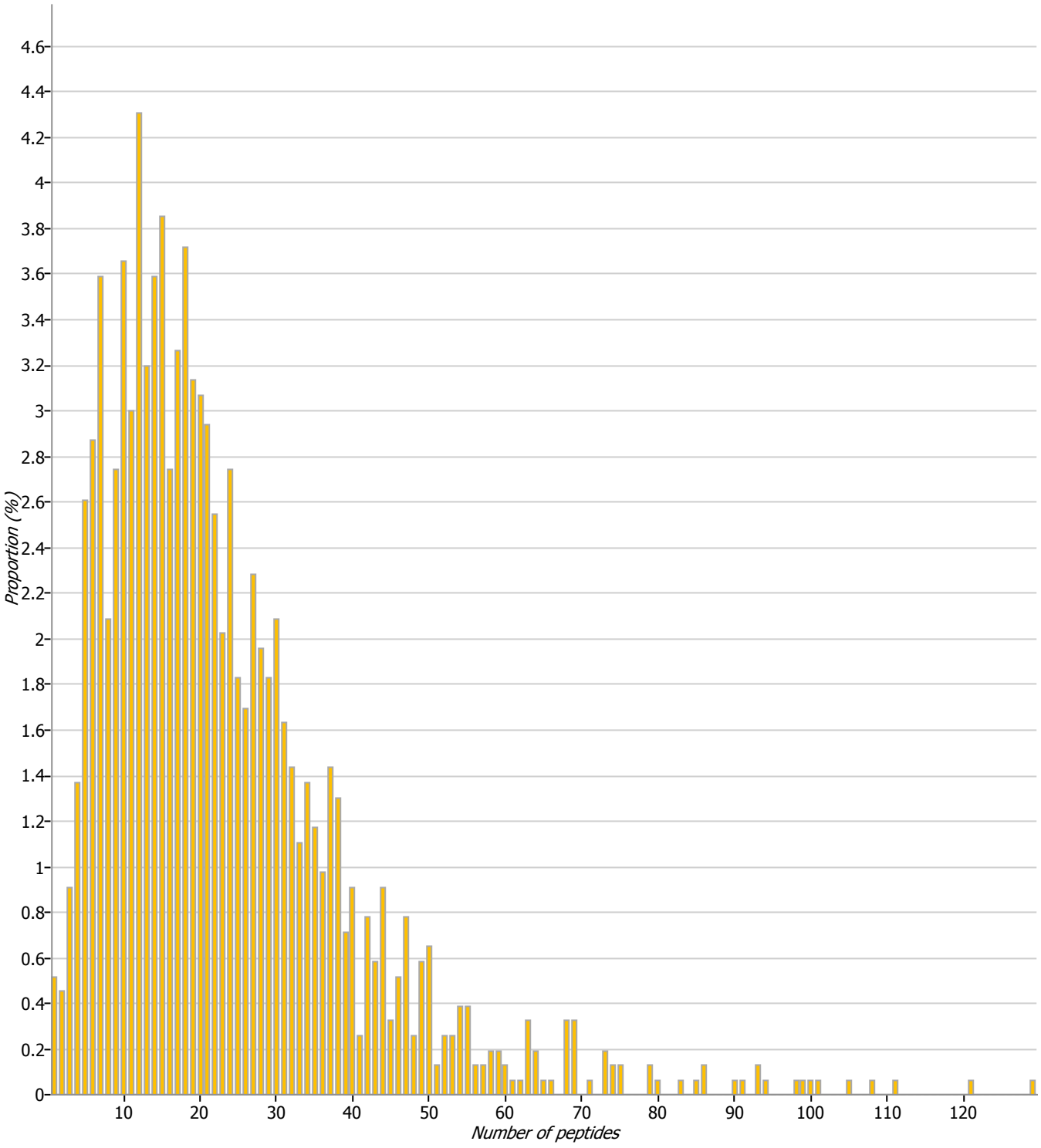


Peptides per protein (overview)

This chart shows the proportional distribution of the number of peptides identified per protein, combined across all runs in the experiment. For an alternative visualisation dividing these data by experimental condition, see the *Peptides per protein (by condition)* metric.

Potential problems:

- An unexpected bias to high or low numbers of peptides may indicate problems with sample preparation or peptide search settings.

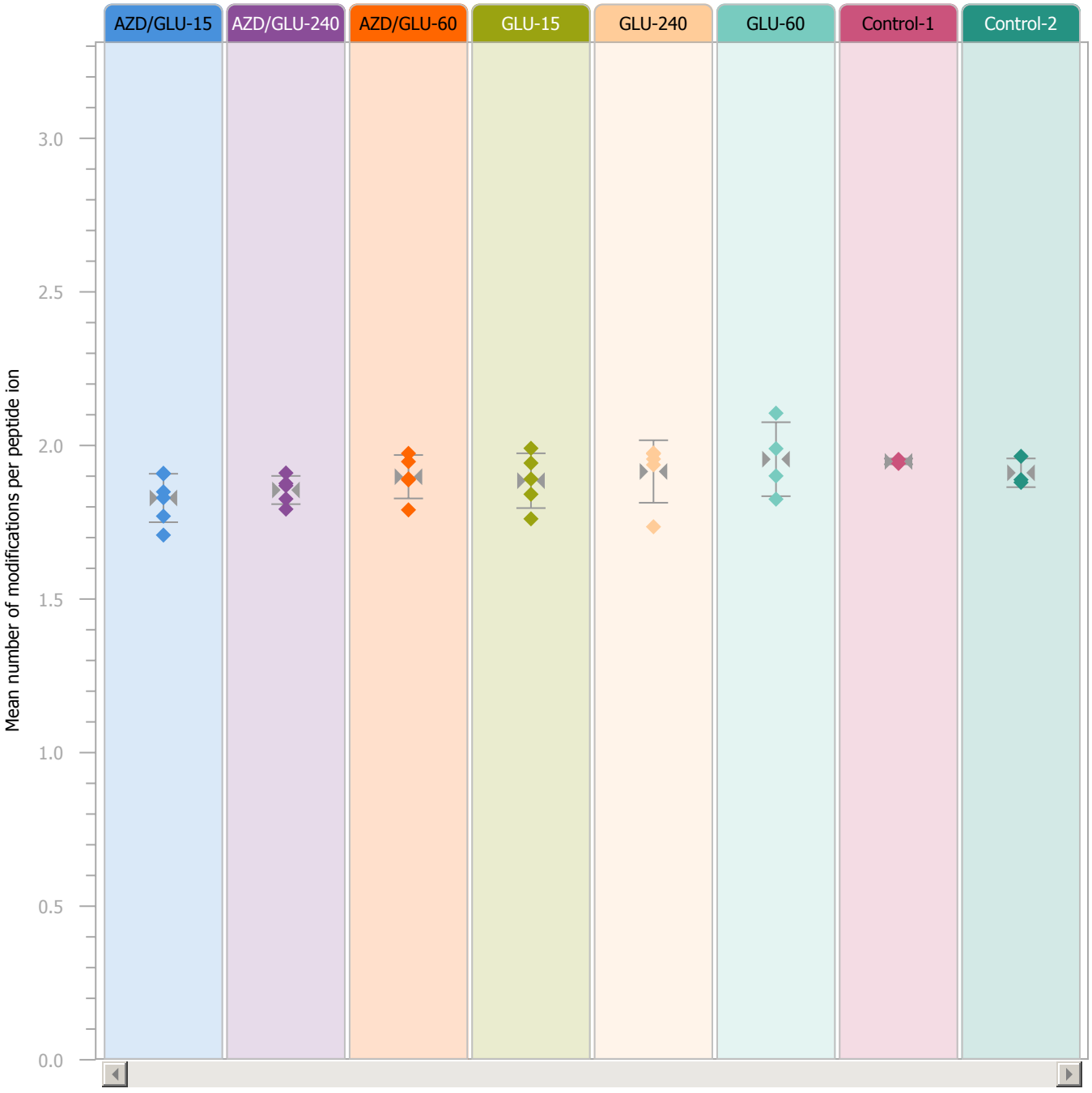


Modifications

The chart below shows the mean number of modifications per peptide ion for runs in the selected experiment design, based on each peptide ion's highest scoring identification. Each run is coloured according to its experimental condition.

Potential problems:

- Unexpectedly low numbers of modifications may indicate that one or more modifications were mistakenly not selected when searching for identifications.
- Variable numbers of modifications across the runs, especially within a given condition, may indicate problems with sample preparation.



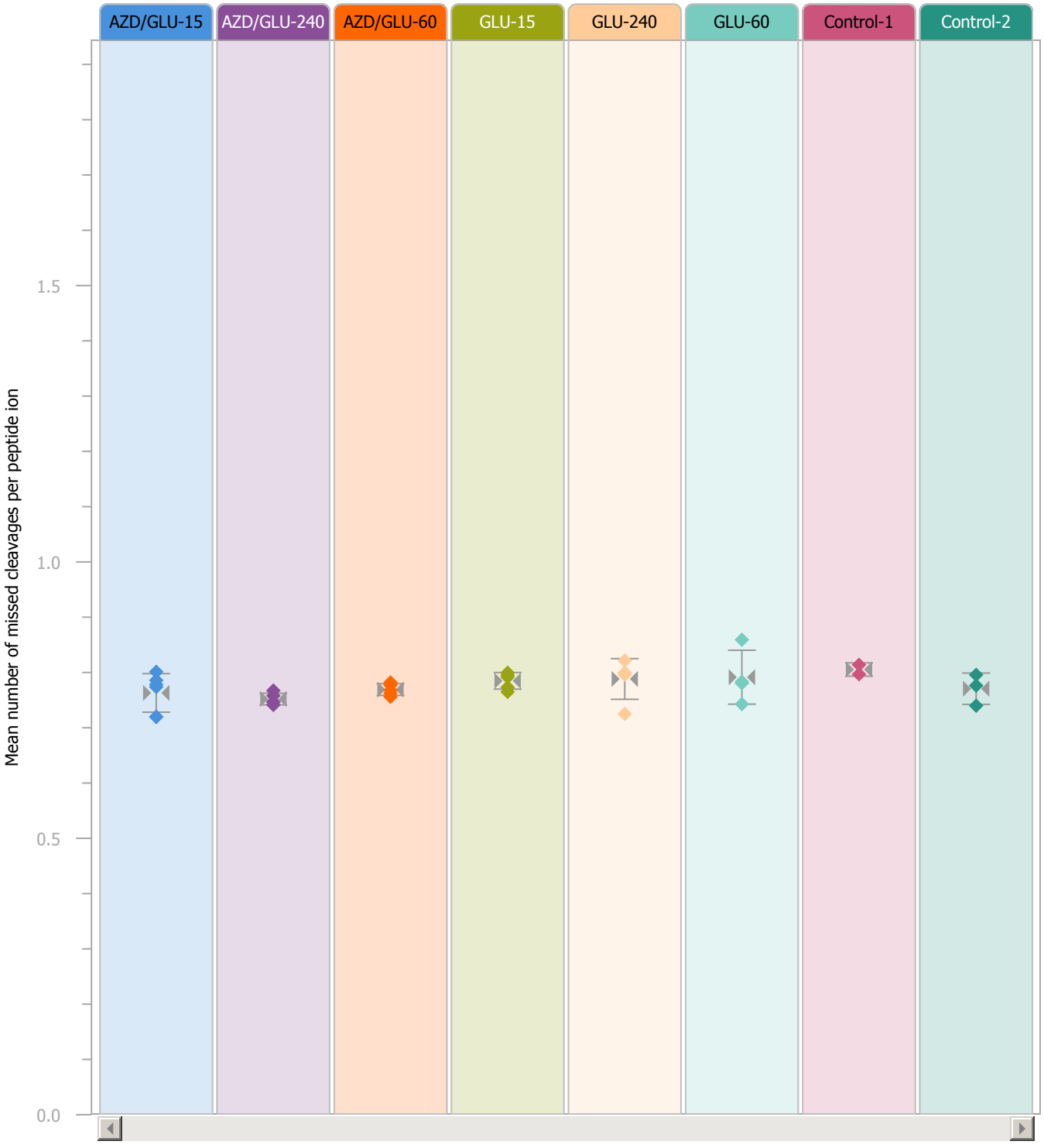
Included modifications Acetyl (Protein N-term) Carbamidomethyl (C) Oxidation (M) Phospho (ST)

Missed cleavages

The chart below shows the mean number of missed cleavages per peptide ion for runs within the selected experiment design, based on each peptide ion's highest scoring identification. The chart assumes the use of trypsin for digestion. Each run is coloured according to its experimental condition.

Potential problems:

- A high number of missed cleavages may indicate problems in trypsinization.
- An absence of missed cleavages may indicate that database search parameters were too stringent.



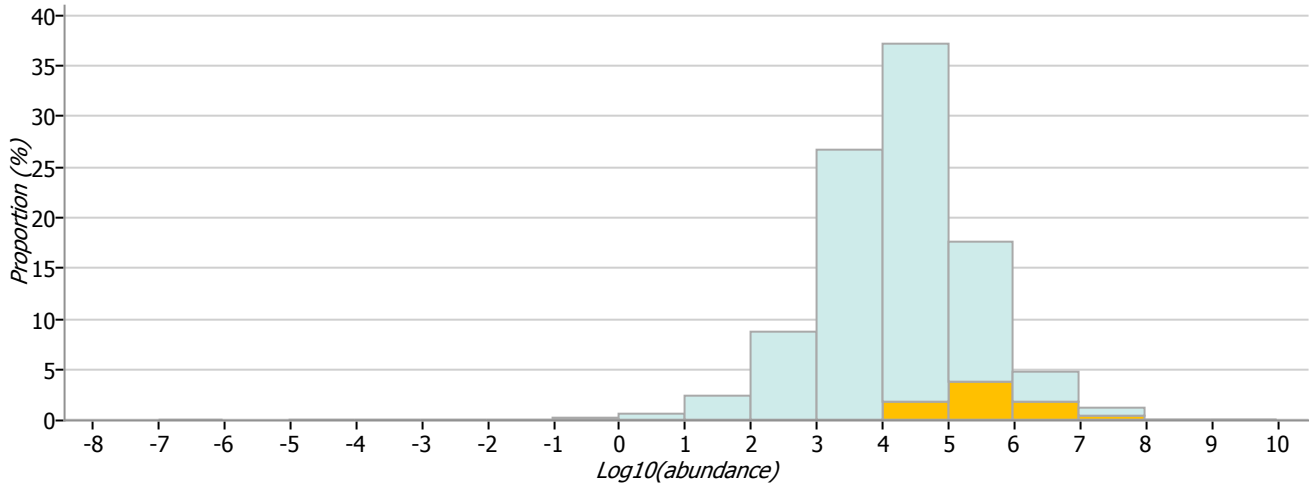
Abundance dynamic range

The charts below show abundance histograms for peptide ions, calculated using the current experiment design. Each chart shows the mean abundance for peptide ions within an experimental condition's runs. Data are binned by Log10 of their normalised abundance and shown as a proportion of the total. Identified peptide ions are shown in yellow.

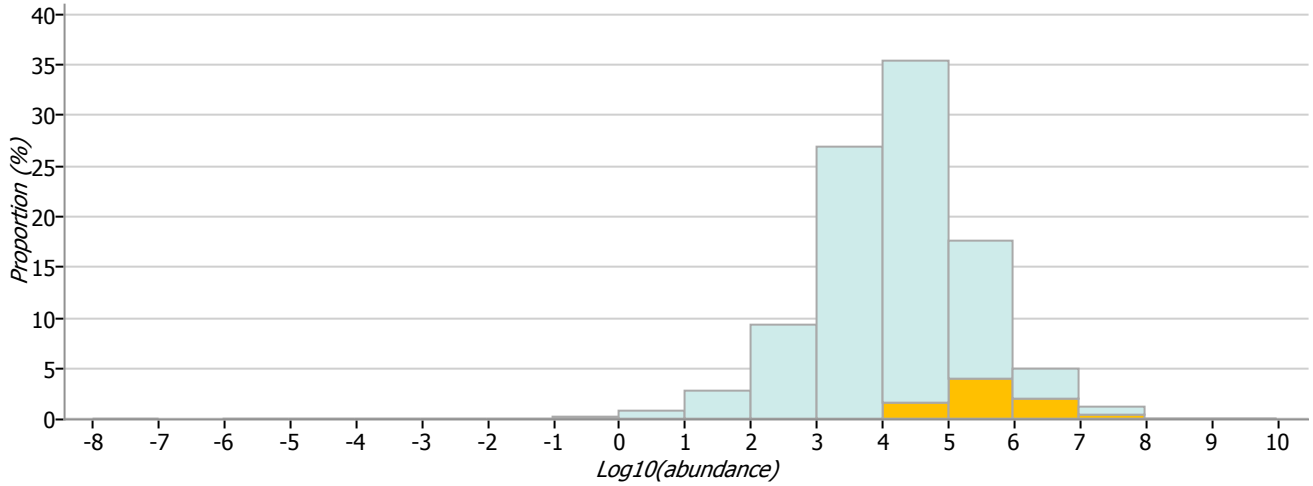
Potential problems:

- A heavily right-skewed histogram of *identified* peptide ions indicates you may be missing identifications with low abundance.
- A heavily right skewed total (summed identified and unidentified) histogram may indicate saturation at high abundance, which will affect the accuracy of quantitation.

AZD/GLU-15

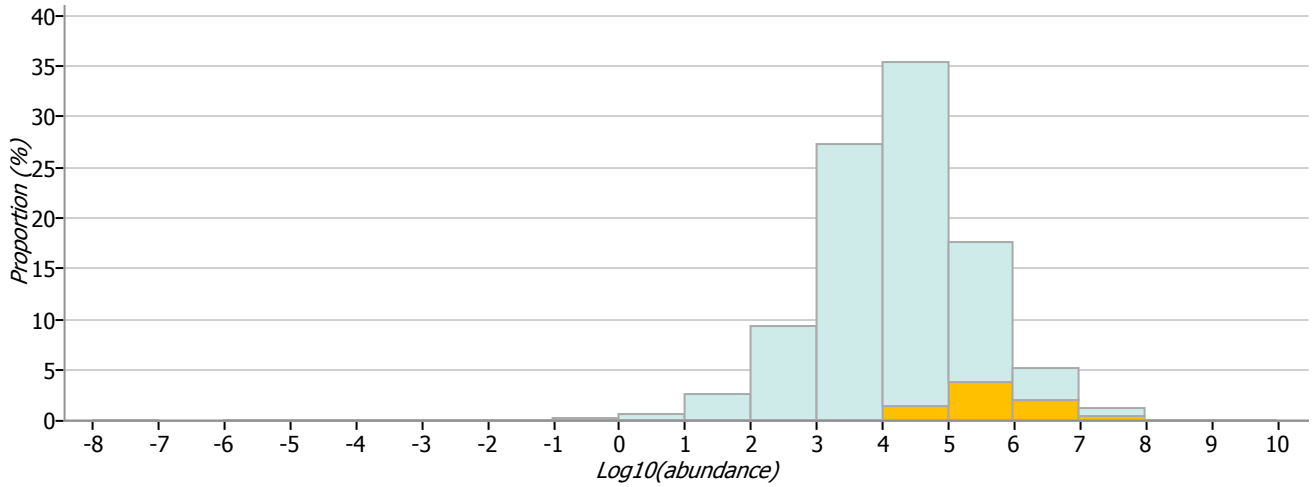


AZD/GLU-240

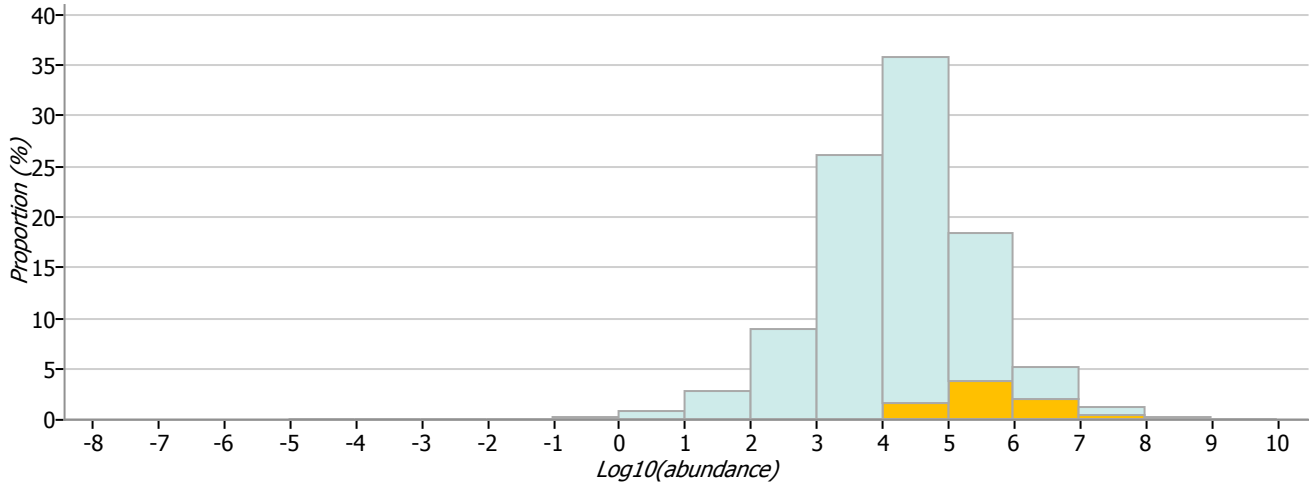


Not identified Identified

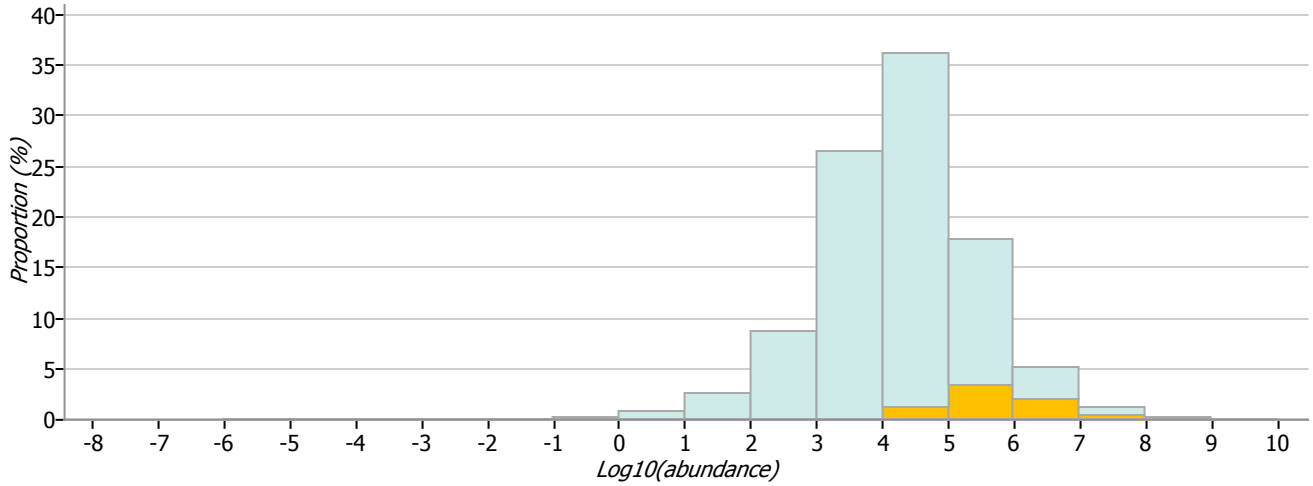
AZD/GLU-60



GLU-15

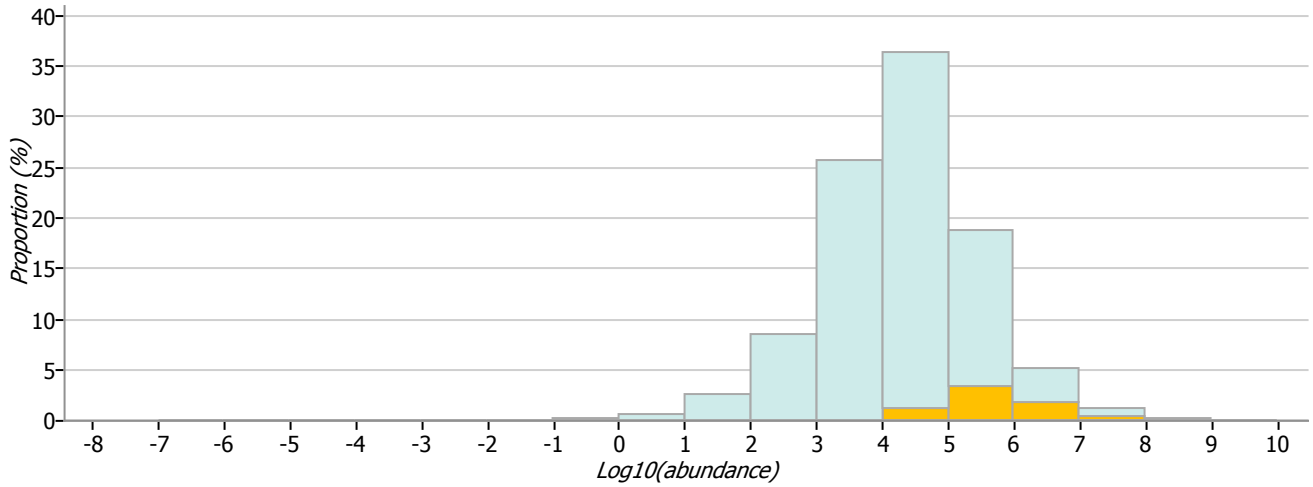


GLU-240

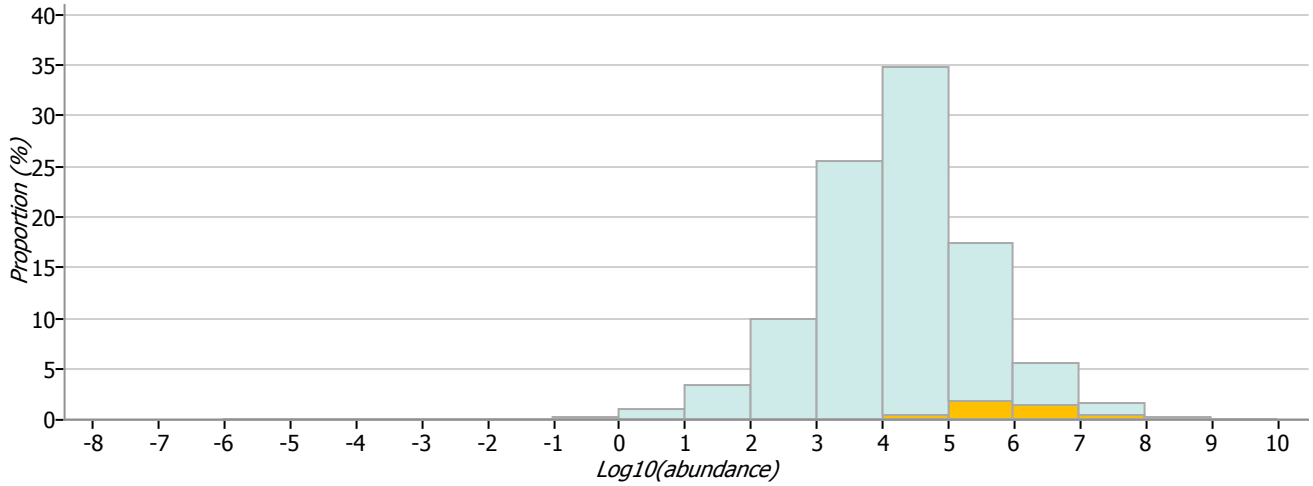


Not identified Identified

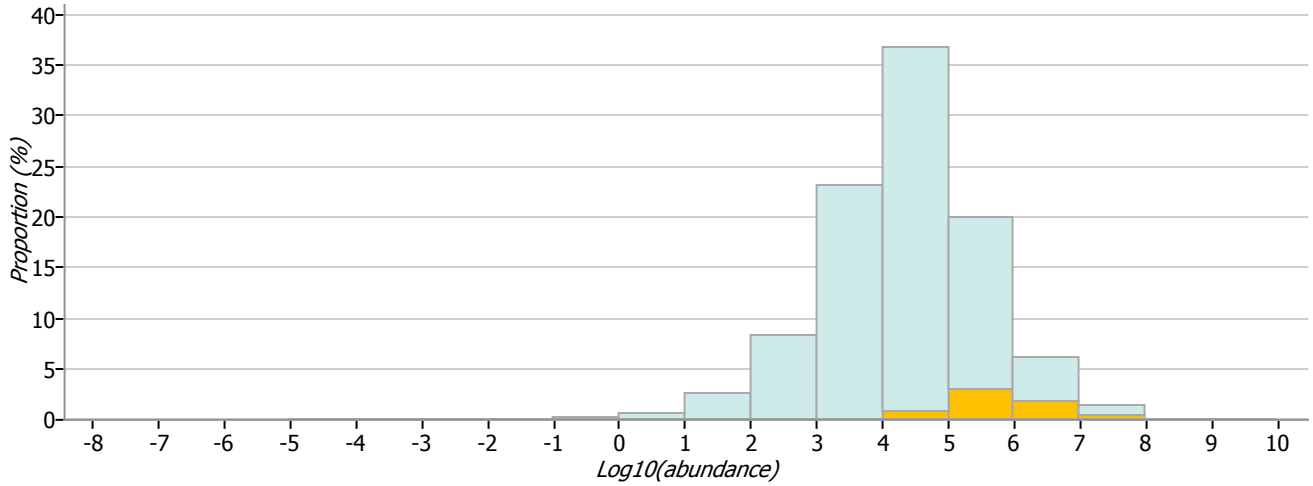
GLU-60



Control-1



Control-2



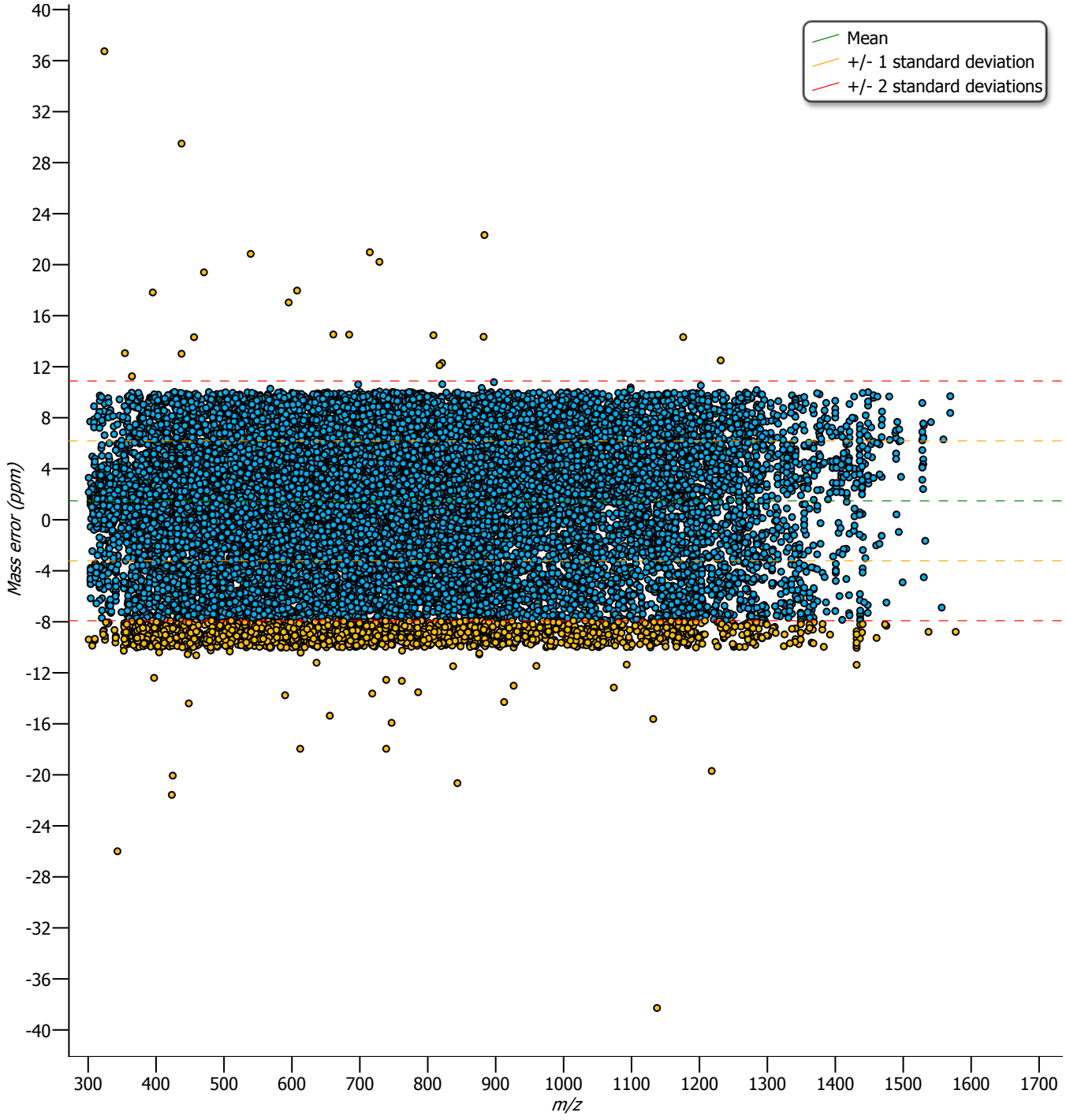
Not identified Identified

Mass accuracy

The chart below shows all identified peptide ions in your experiment, plotting peptide ion m/z against the ppm error in its highest scoring identification. Blue points indicate peptide ions which have a mass error within 2 standard deviations of the mean, yellow points indicate peptide ions with a mass error more than 2 standard deviations from the mean.

Potential problems:

- A dependence of ppm mass error on m/z may indicate poor calibration.
- If the standard deviation of the data is large in ppm terms, this may indicate that your search parameters are too lenient.



Scan rates

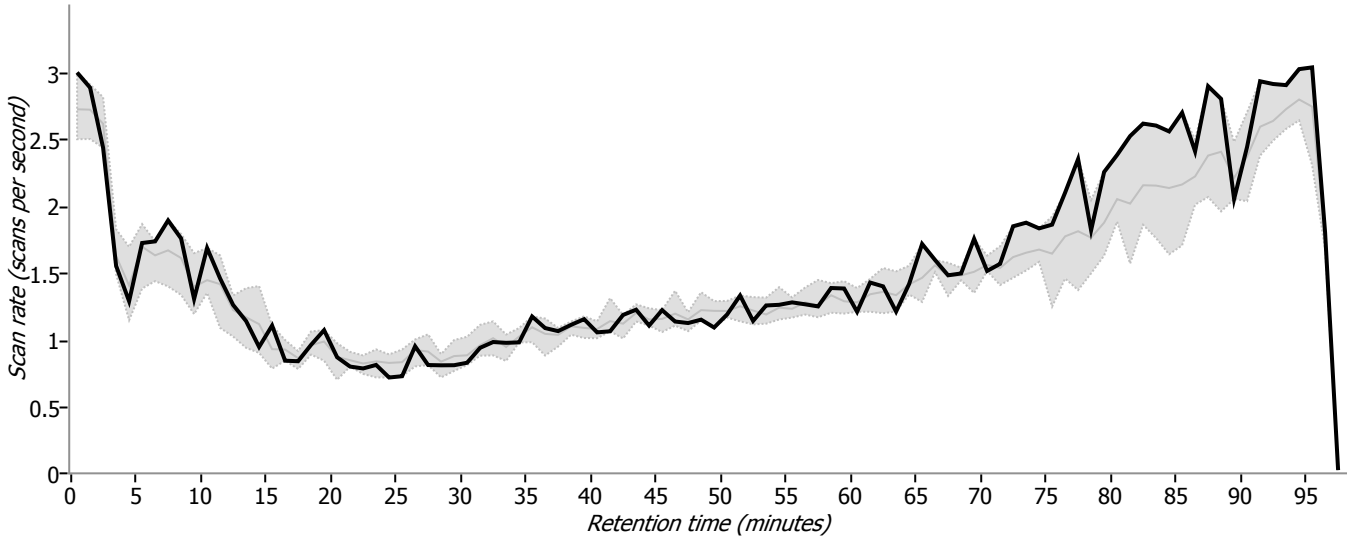
The charts below show the MS1 scan rate over the duration of your runs, using the current experiment design. Each chart shows the scan rate variation within an experimental condition's runs. The named run is highlighted in black. The variability between runs is shown as a grey area. The y-axis shows scans per second in a 30-second window centred on each x-axis time point.

Potential problems:

- A highly varying scan rate means quantitation accuracy may be negatively affected.

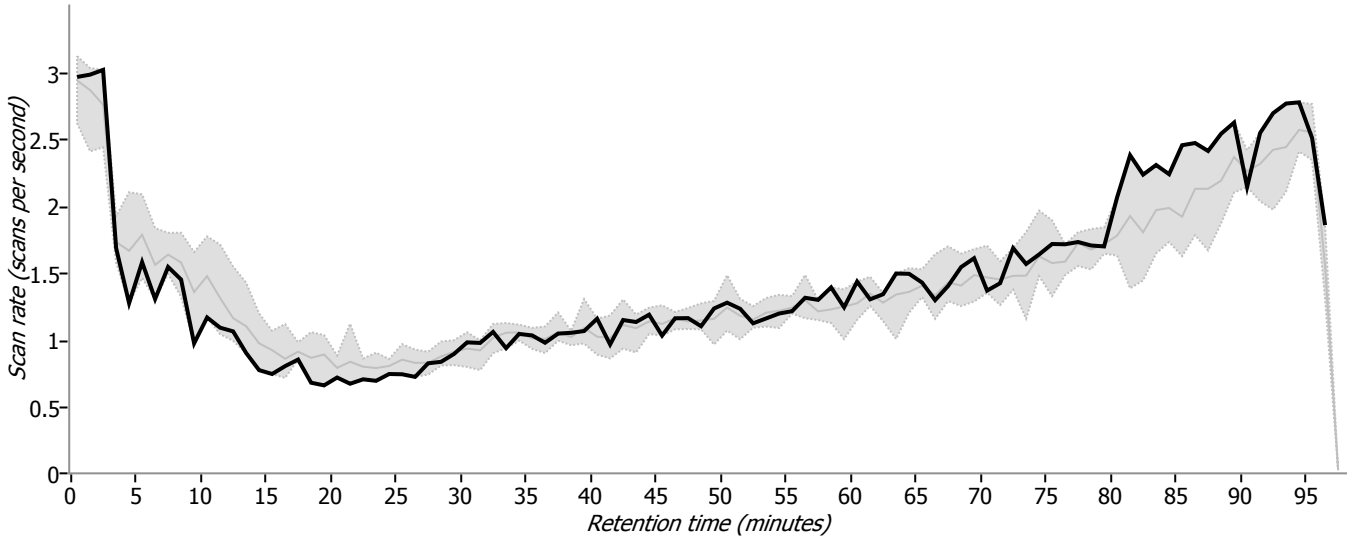
AZD/GLU-15

Run: 7



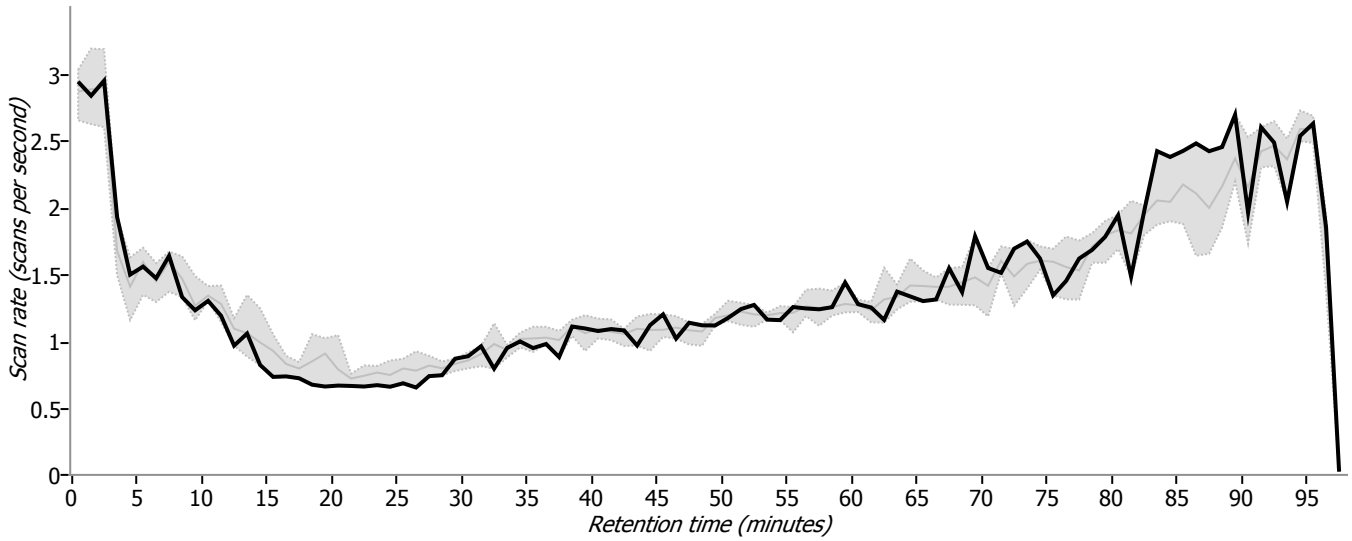
AZD/GLU-240

Run: 2



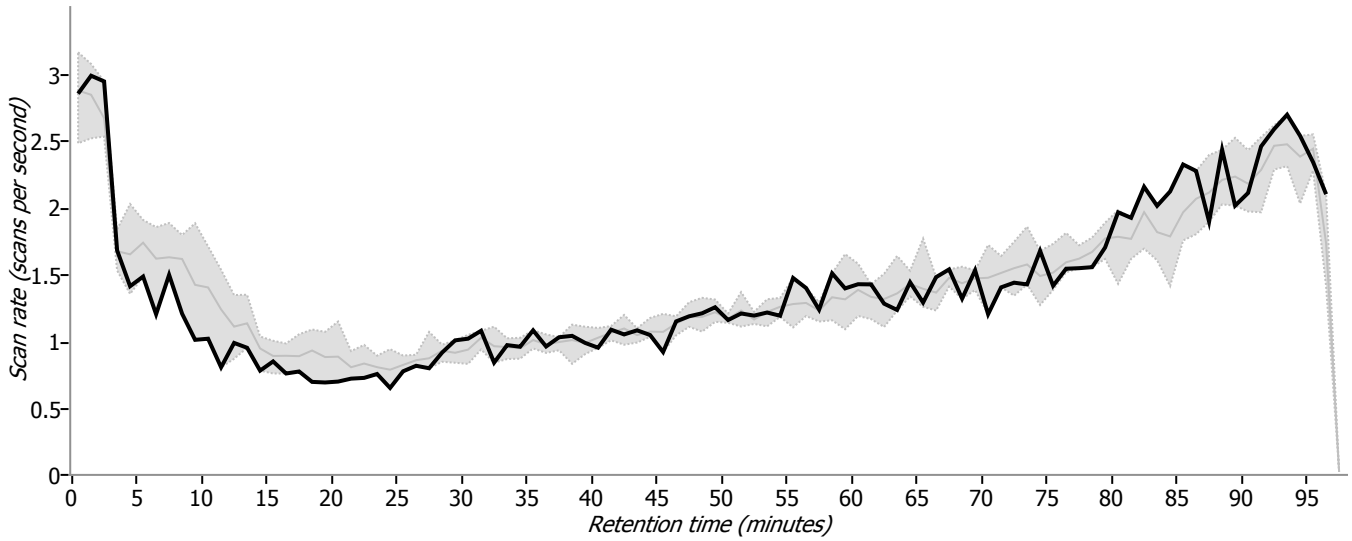
AZD/GLU-60

Run: 3



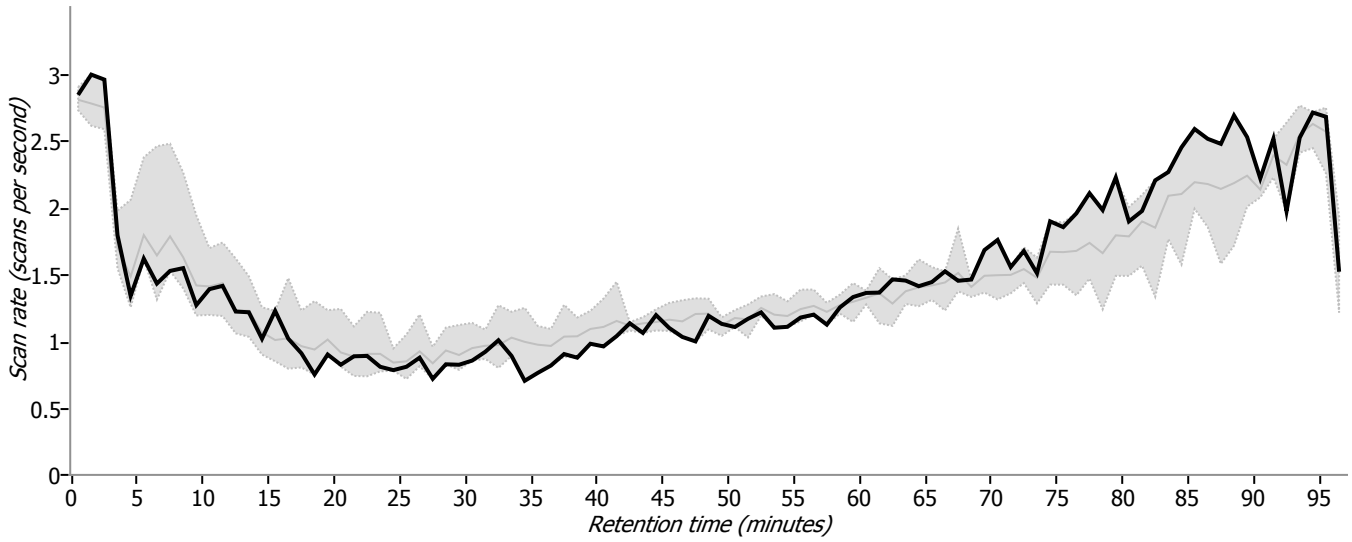
GLU-15

Run: 4



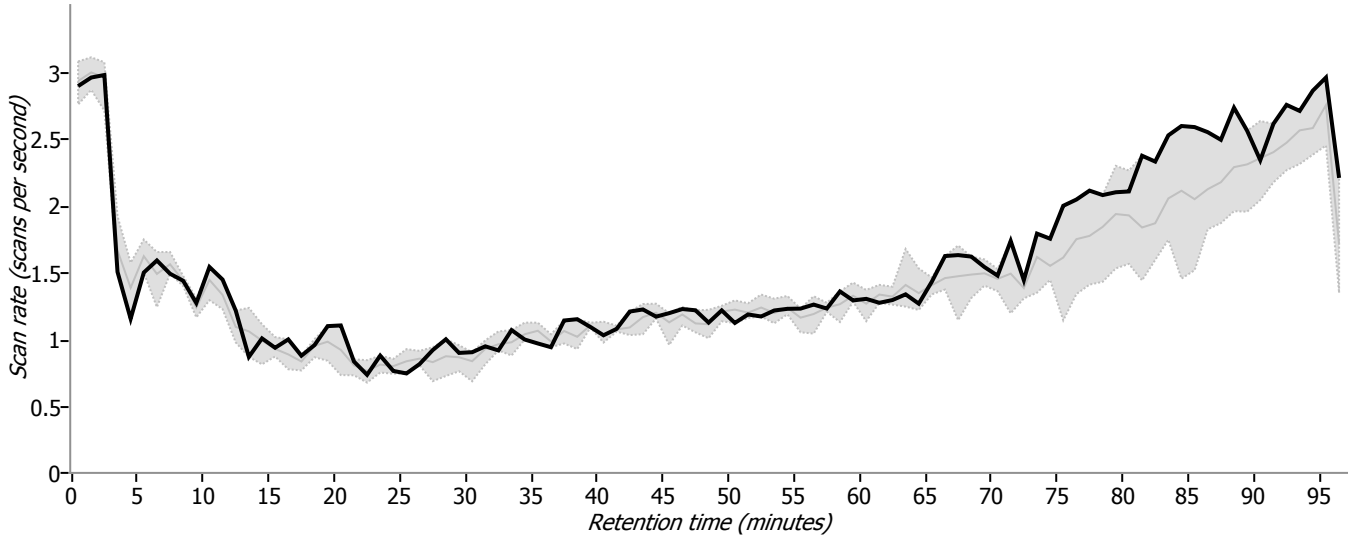
GLU-240

Run: 5



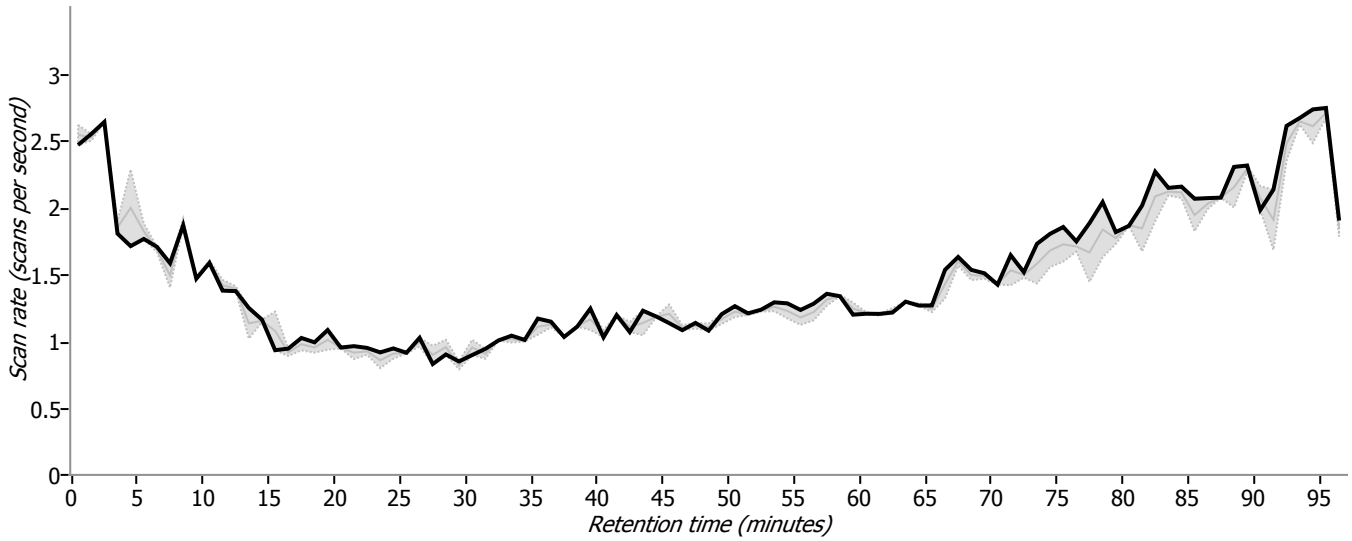
GLU-60

Run: 23



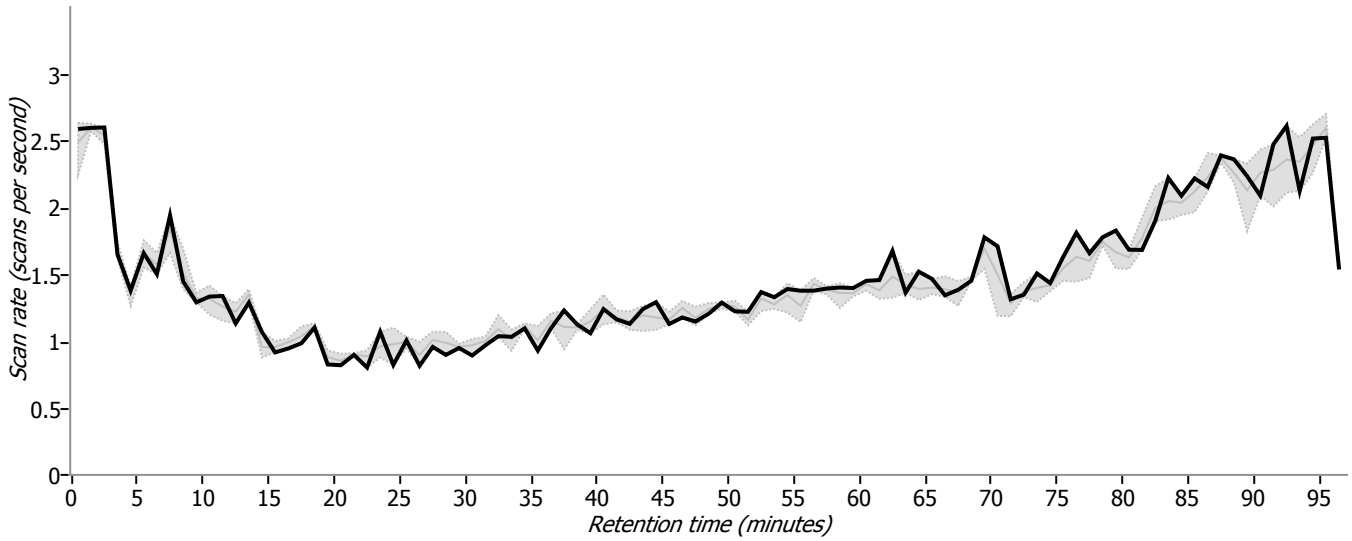
Control-1

Run: A



Control-2

Run: i

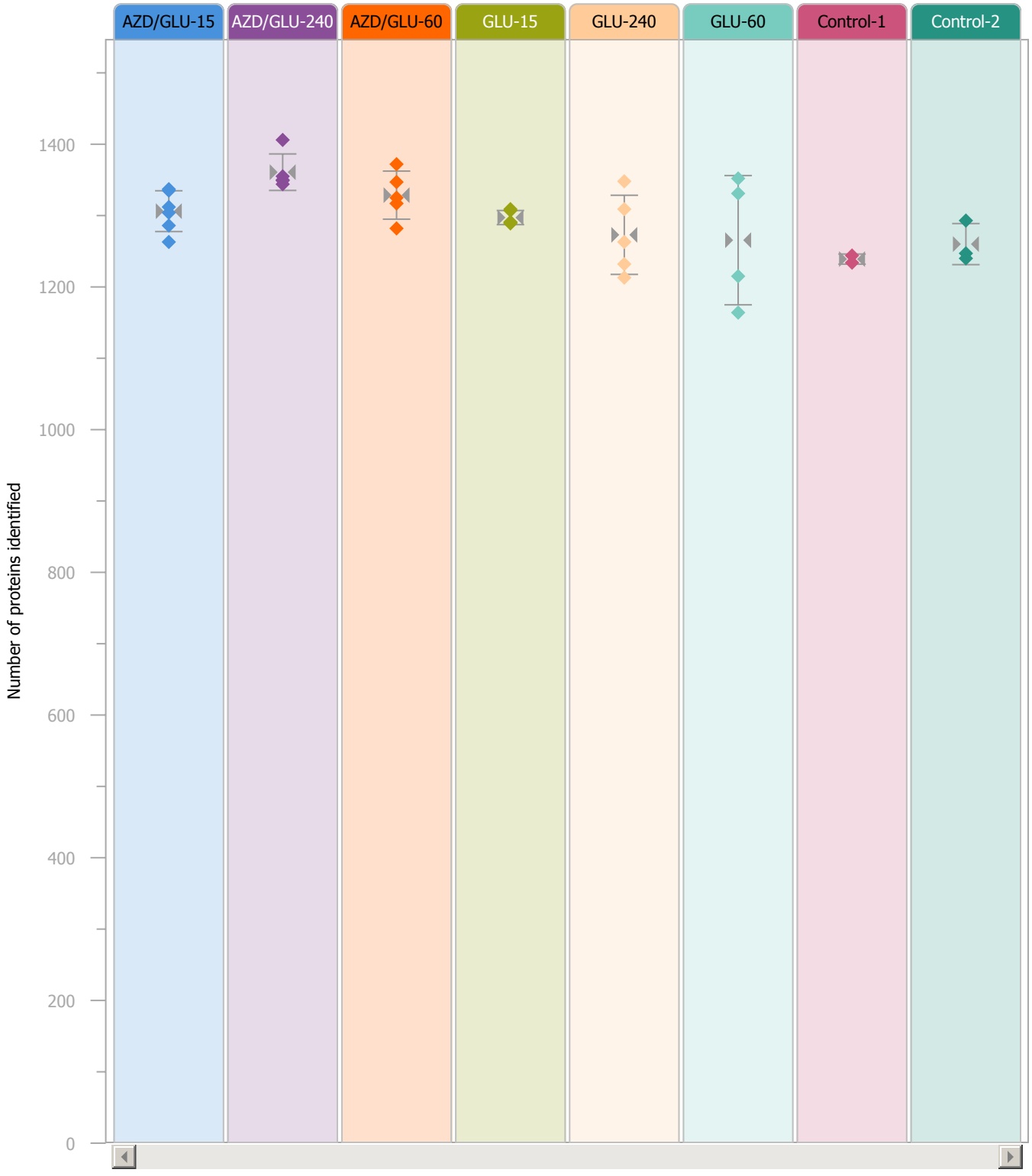


Proteins

The chart below shows the number of proteins identified in each of the runs within the selected experiment design. Each run is coloured according to its experimental condition.

Potential problems:

- Any exceptionally high or low values may indicate problems with sample preparation, chromatography, or instrument settings.

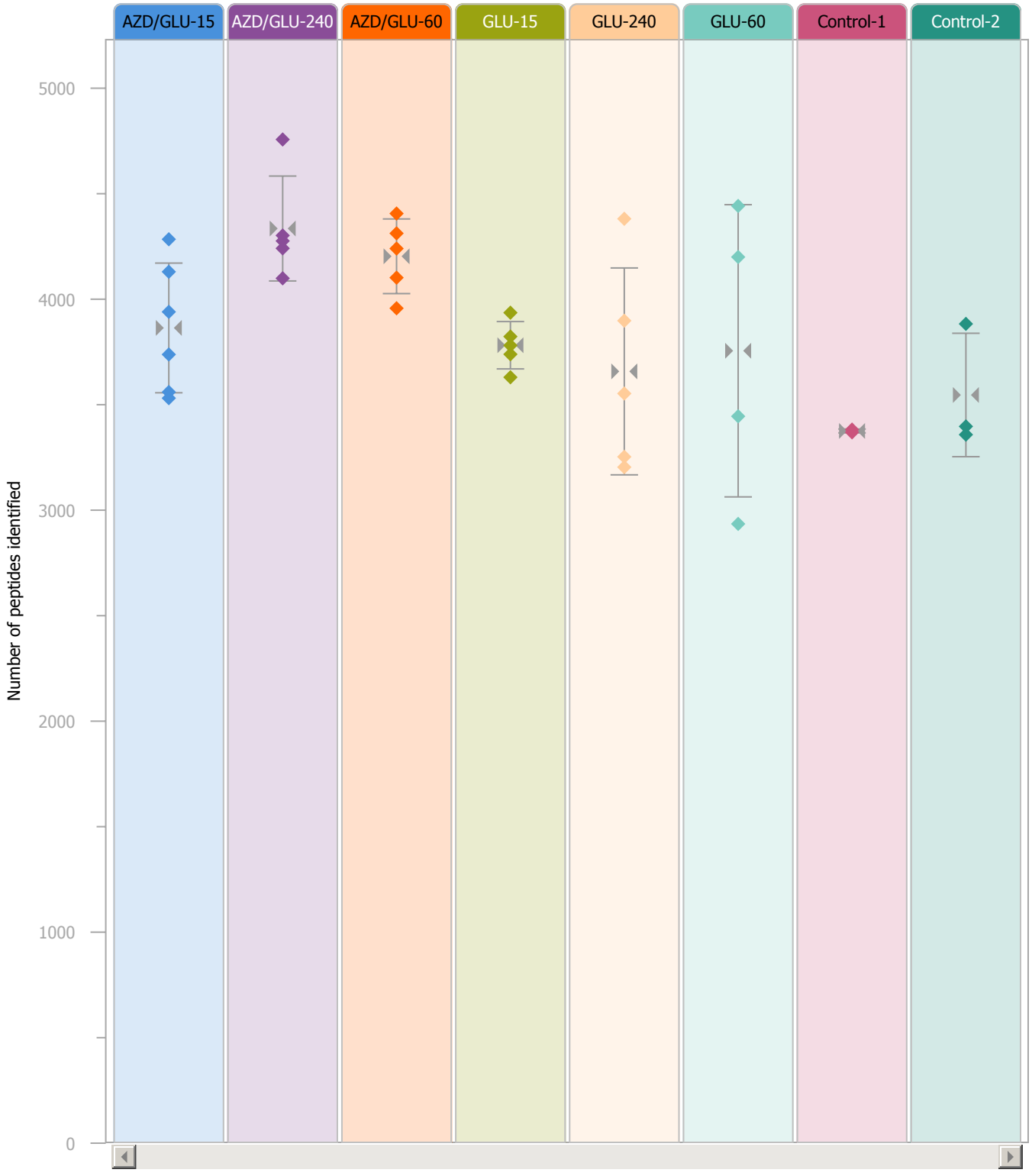


Peptides

The chart below shows the number of peptides identified in each of the experiment's runs. Each run is coloured according to its experimental condition.

Potential problems:

- Any exceptionally high or low values may indicate problems with sample preparation, chromatography, or instrument settings.

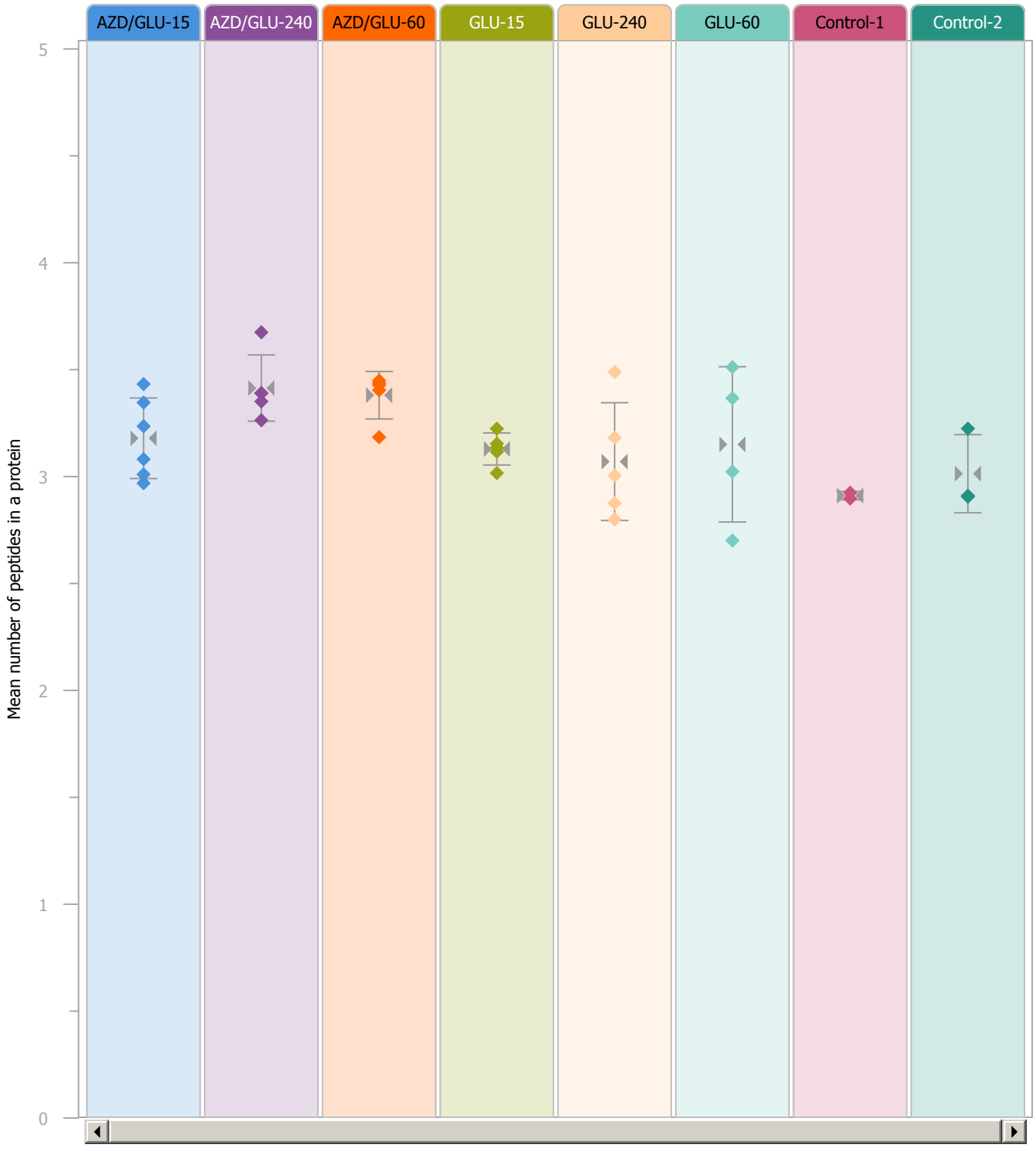


Peptides per protein (by condition)

The chart below shows the average number of peptides per protein in each run within the selected experiment design. For a given run, the value shown is calculated using only identifications from that run.

Potential problems:

- Any exceptionally high or low values may indicate problems with sample preparation or peptide search settings.

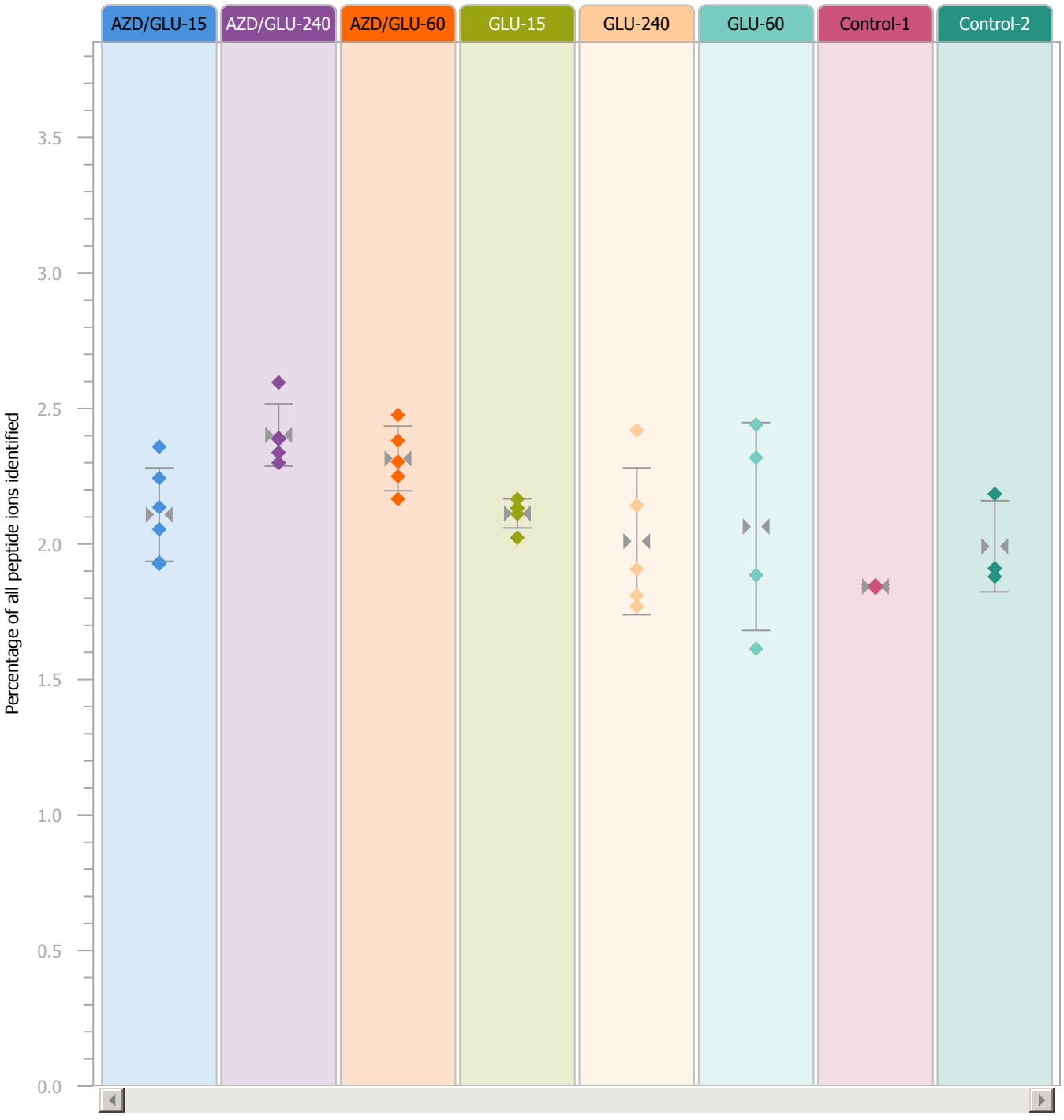


Percentage of peptide ions identified

The chart below shows the number of peptide ions identified in each of the runs within the selected experiment design, expressed as a percentage of the total number of peptide ions. Each run is coloured according to its experimental condition.

Potential problems:

- Any exceptionally high or low values may indicate problems with sample preparation, chromatography, or instrument settings.
- Very low values across all runs may indicate a problem with the database that was searched for identifications, or with other search parameters.



Protein overlap

The Venn diagram shows the number of proteins identified uniquely in the selected conditions and the number that are shared between conditions. Use the list on the right to select two or three conditions to explore.